On the nonlocality of the fractional Schrödinger equation

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A number of papers over the past eight years have claimed to solve the fractional Schrödinger equation for systems ranging from the one-dimensional infinite square well to the Coulomb potential to one-dimensional scattering with a rectangular barrier. However, some of the claimed solutions ignore the fact that the fractional diffusion operator is inherently nonlocal, preventing the fractional Schrödinger equation from being solved in the usual piecewise fashion. We focus on the one-dimensional infinite square well and show that the purported groundstate, which is based on a piecewise approach, is definitely not a solution of the fractional Schrödinger equation for general fractional parameters $\alpha$. On a more positive note, we present a solution to the fractional Schrödinger equation for the one-dimensional harmonic oscillator with $\alpha = 1$.

I. INTRODUCTION

A wide variety of stochastic processes are more general than the familiar Brownian motion, but presumably can still be described by modifying the diffusion equation using a fractional Laplacian operator \cite{1, 2}. Such “fractional diffusion” is now a large and active field, and a number of books have been written on the mathematics and physics of fractional diffusion operators \cite{3, 4, 5}. In 2000, Laskin introduced the fractional Schrödinger equation, in which the normal Schrödinger equation is modified in analogy with fractional diffusion \cite{6, 7, 8}. Laskin claimed to exactly solve this equation in the case of the one-dimensional infinite square well \cite{6}. A more recent (2006) work claimed to find solutions again for the infinite one-dimensional square well (agreeing with Laskin’s original solution), and for one-dimensional scattering off of a barrier potential \cite{9}. A 2007 work used a different method of analysis to claim solutions for the linear, delta function, and Coulomb potentials in one dimension \cite{10}. Laskin also recently built on the same claimed solution to derive properties of the quantum kernel \cite{11}. The purpose of this work is to point out that of the many purported exact solutions presented in the literature, only the one for the delta function potential is correct.

The one-dimensional fractional Schrödinger equation \cite{6} is

\[ i\hbar \frac{\partial \psi(x,t)}{\partial t} = D_\alpha (-\hbar^2 \Delta)^{\alpha/2} \psi(x,t) + V(x,t) \psi(x,t), \]

(1)

where $D_\alpha$ is a constant, $\Delta \equiv \partial^2/\partial x^2$ is the Laplacian, and $(-\hbar^2 \Delta)^{\alpha/2}$ is the quantum Riesz fractional derivative:

\[ (-\hbar^2 \Delta)^{\alpha/2} \psi(x,t) = \frac{1}{2\pi\hbar} \int_{-\infty}^{+\infty} dp \ e^{ipx/\hbar} \ |p|^{\alpha} \ \phi(p,t). \]

(2)

Here, $\phi(p,t)$ is the Fourier transform of the wavefunction,

\[ \phi(p,t) = \int_{-\infty}^{+\infty} dx \ \psi(x,t) e^{-ipx/\hbar}. \]

(3)

When $\alpha = 2$, the quantum Riesz fractional derivative becomes equivalent to an ordinary Laplacian, and we recover the ordinary Schrödinger equation.

We focus on the case where the potential is independent of time, so we are interested in solutions of the following equation:

\[ D_\alpha (-\hbar^2 \Delta)^{\alpha/2} \psi(x) + V(x) \psi(x) = E \psi(x). \]

(4)
The fractional diffusion operator is a nonlocal operator except when $\alpha = 0, 2, 4, \ldots$. This means that $(-\hbar^2 \Delta)^{\alpha/2} \psi(x)$ depends not just on $\psi(y)$ for $y$ near $x$, but on $\psi(y)$ for all $y$. This nonlocality, in turn, means that when solving Eq. (4), the form of the wavefunction in a given region depends not just on the potential in that region, but on the potential everywhere. Because of this, for a piecewise-defined potential, we cannot follow the normal strategy of solving separately for the wavefunction in each piecewise region, and then using conditions of continuity and differentiability to match up the solutions. However, this is precisely the strategy used in the papers cited above, and the solutions obtained in those papers are thus invalid. We illustrate the problem by looking in some detail at the case of the one-dimensional infinite square well in Section II. The problems with the purported solutions for other potentials are similar, and are discussed in Section III. Section IV presents an exact solution for the one-dimensional fractional harmonic oscillator with $\alpha = 1$, followed by conclusions in Section V.

II. INFINITE ONE-DIMENSIONAL SQUARE WELL

Consider Eq. (4) in the limit of the potential becoming an infinite square well

$$V(x) = \begin{cases} 0 & \text{if } |x| < a \\ \infty & \text{if } |x| \geq a. \end{cases}$$

We first note that for the case of free space, where the potential $V$ is zero everywhere, it is easy to see that plane waves are eigenfunctions of the quantum fractional Hamiltonian:

$$(-\hbar^2 \Delta)^{\alpha/2} e^{ipx/\hbar} = |p|^\alpha e^{ipx/\hbar}. \quad (6)$$

However, Eq. (6) is only valid if the function operated on is $e^{ipx/\hbar}$ everywhere; it is not a local equation that can be applied just in a restricted region. Because the quantum Riesz fractional derivative is a nonlocal operator, the wavefunction in the well knows about the wavefunction and potential outside of the well. Previous works looking at the one-dimensional infinite square well incorrectly applied Eq. (6) only inside the well, and concluded that the solution inside the well would be a simple linear superposition of left- and right-moving plane waves of the same energy [6, 9].

Although these papers use an invalid assumption, could their end results be correct nevertheless? Both papers claim that the solutions for the one-dimensional square well are the same for the fractional case as for the standard non-fractional case, only with modified energies. So, they obtain for the ground state

$$\psi_0(x) = \begin{cases} A \cos \left( \frac{\pi x}{2a} \right) & \text{for } |x| \leq a \\ 0 & \text{otherwise}. \end{cases} \quad (7)$$

The Fourier transform of this is

$$\phi_0(p) := \int_{-\infty}^{+\infty} dx \, e^{-ipx/\hbar} \psi_0(x),$$

$$= -\frac{A \pi \hbar^2}{a} \frac{\cos (ap/\hbar)}{p^2 - (\pi \hbar/2a)^2}. \quad (8)$$

From $\phi_0(p)$ we can calculate the fractional Riesz derivative:

$$(-\hbar^2 \Delta)^{\alpha/2} \psi_0(x) = -\frac{2A}{\pi} \left( \frac{\pi \hbar}{2a} \right)^{\alpha} \int_0^\infty dp \, \frac{p^{\alpha}}{p^2 - 1} \cos \left( \frac{1}{2} \pi p \right) \cos \left( \frac{\pi px}{2a} \right). \quad (9)$$

We see here how the nonlocality manifests itself in the mathematics. If we only looked at the wavefunction inside the square well, then $\psi_0(x)$ would appear to consist of plane waves of just two wavevectors, $\pm \pi/(2a)$. However, in reality, $\psi_0(x)$ is 0 outside the well, making it a wave packet, rather than just a combination of two plane waves, and so it contains a continuous range of wavevectors, as seen in Eq. (8). The fractional Riesz derivative thus sees all these wavevectors.

Now we shall show that $\psi_0(x)$ is not a solution of the infinite square well via a proof by contradiction. First, assume that $\psi_0(x)$ is a solution of the fractional Schrödinger equation. Then the fractional Riesz derivative $(-\hbar^2 \Delta)^{\alpha/2} \psi_0(x)$ must be proportional to $\psi_0(x)$ on the open interval, $|x| < a$, where $V(x) = 0$. Since, $\psi_0(x)$ is continuous and $\psi_0(a) = 0$, this implies that the limit $x \to a^-$ of (9) should also vanish. However, this condition is not equivalent to (9) vanishing at $x = a$ because the Hamiltonian includes the potential and so we cannot rely on continuity of $\psi_0(x)$ at $x = a$. 
A Fourier transform such as (9) is continuous if the integral is absolutely convergent. The integrand in (9) is bounded by $p^\alpha$ for small $p$ and by $(1 + \epsilon)p^{\alpha - 2}$ for large $p$. Therefore, (9) is indeed a continuous function for all $x$ for $-1 < \alpha < 1$. Thus, for $-1 < \alpha < 1$, we can take the limit $x \to a^-$ (9) by setting $x = a$, and if $\psi_0(x)$ is a solution, this should give zero:

$$f(\alpha) := \int_0^\infty dp \frac{p^\alpha}{p^2 - 1} \cos^2 \left( \frac{1}{2} \pi p \right) = 0.$$  \tag{10}

Taking the derivative with respect to $\alpha$, we see

$$\frac{df}{d\alpha} = \int_0^\infty dp \frac{p^\alpha \ln p}{p^2 - 1} \cos^2 \left( \frac{1}{2} \pi p \right).$$  \tag{11}

The integrand in Eq. (11) is everywhere positive, so $df/d\alpha > 0$, and we cannot have $f(\alpha) = 0$ for all $\alpha$. The ground state (7) claimed in Refs. [6] and [9] thus cannot be a solution of the fractional Schrödinger equation for all $\alpha$. It can only be a solution once in the interval $-1 < \alpha < 1$—namely when $\alpha = 0$.

The above argument does not hold for $1 \leq |\alpha|$ and in fact for some values of $\alpha$, (9) is not continuous at $x = a$. However, a related argument to one presented above shows that this $\psi_0$ cannot be a solution at least for $1 < \alpha < 2$. For $\alpha = 2$, on the other hand, $\psi_0(x)$ actually is a solution. Indeed it is a solution whenever the fractional Riesz derivative is an ordinary derivative—that is, for $\alpha = 0, 2, 4, \ldots$.

It may seem counterintuitive that Eq. (7) is not the correct ground state. The standard ($\alpha = 2$) Schrödinger equation for an infinite potential well is equivalent to the Schrödinger equation on an interval with the Dirichlet boundary conditions $\psi(-a) = \psi(a) = 0$. By raising that Hamiltonian to the power $\alpha/2$ we get a plausible fractional Laplacian and Eq. (7) is indeed a solution. However, this is not the Riesz fractional derivative. In other words, the fractional Schrödinger equation for an infinite potential well is not equivalent to the fractional Schrödinger equation on an interval.

At this point, we do not know what the true solutions are for values of $\alpha$ other than $0, 2, 4, \ldots$. In Ref. [12], Zoia et al. find numerical solutions for the ground state. The solutions depend on $\alpha$ and differ from the simple sine wave solution in Eq. (7).

III. OTHER SYSTEMS

While we have only discussed the infinite one-dimensional square well in detail, the comments here equally invalidate the other claimed solutions of the fractional Schrödinger equation. For example, in Section II of Ref. [10], the linear potential,

$$V(x) = \begin{cases} Fx & \text{if } x \geq 0 \\ \infty & \text{if } x < 0 \end{cases},$$  \tag{12}

is studied. The authors of Ref. [10] treat this equation in a piecewise approach by solving the equation for the potential $V(x) = Fx$ and applying a boundary condition at $x = 0$. This is invalid for the same reasons stated above for the square well potential. Similar comments apply to the analysis of the Coulomb potential in section IV of that same paper.

Our comments, however, do not invalidate the analysis of the delta function potential in Section III of Ref. [10], which did not implement a piecewise approach, but instead worked with the Fourier transform of the delta function potential. However, the authors of Ref. [10] fail to note that the bound state for the delta function potential is valid only for $\alpha \geq 1$. For $\alpha < 1$, there is no bound state since the integral in Eq. 33 of Ref. [10] diverges. In more recent work, Dong and Xu [13] attempt to solve the same problem again, using a piecewise approach. They then compare this to their initial correct solution and derive an incorrect identity for the H-function.

IV. THE FRACTIONAL HARMONIC OSCILLATOR

Consider the fractional Schrödinger equation with the potential

$$V(x) = \frac{1}{2} k x^2.$$  \tag{13}
Fourier transforming Eq. (11) gives
\[ \frac{1}{2} \hbar^2 \frac{d^2 \phi}{dp^2} = (D_\alpha |p|^{\alpha} - E)\phi(p). \] (14)
In momentum space, the equation maps to the ordinary Schrödinger equation with a positive \( \alpha \) power law potential and \( k = 1/m \). In other words, the kinetic and potential energies have reversed roles.

### A. WKB approximation

Given the mapping to ordinary quantum mechanics, in the limit \( \hbar \to 0 \), one can use the WKB approximation in momentum space to approximate the energy eigenvalues, with \( p \) replacing \( x \). The quantization condition in momentum space is
\[ \int_{p_1}^{p_2} \lambda(p) dp = \left( n + \frac{1}{2} \right) \pi \hbar, \quad n \in \{0\} \cup \mathbb{Z}^+, \] (15)
where \( \lambda(p) = \sqrt{\frac{2}{k}(E - D_\alpha |p|^{\alpha})} \), and \( p_1 \) and \( p_2 \) are the classical turning points, i.e. \( p_{1,2} = \pm (E/D_\alpha)^{1/\alpha} \). The above condition leads to
\[ E_n = -\left( \frac{\left( n + \frac{1}{2} \right) \pi \sqrt{k(D_\alpha)^{1/\alpha}}}{2\sqrt{2}\Gamma\left(\frac{3}{2} + \frac{1}{\alpha}\right)} \right)^{2/\alpha} \left( \frac{k}{2} \hbar^2 D_1^2 \right)^{1/3} r_n. \] (16)
This agrees with Laskin’s more general WKB result \cite{14} for an arbitrary power-law potential. However, by the argument we have just given, this special case is better justified than Laskin’s general claim. It is unclear whether there is any reason to believe the WKB approximation to be valid for systems other than the harmonic oscillator, since for other potentials, the Fourier transform of the fractional Schrödinger equation will not be an ordinary Schrödinger equation.

### B. An exact solution for \( \alpha = 1 \)

When \( \alpha = 1 \), Eq. (11) becomes
\[ \frac{1}{2} \hbar^2 \frac{d^2 \phi}{dp^2} = (D_1 |p| - E)\phi(p). \] (17)
Restricting to \( p > 0 \) or \( p < 0 \), this differential equation is equivalent to the Airy equation (by a rescaling transformation). For a normalizable wavefunction, we must have \( \phi(p = \infty) = \phi(p = -\infty) = 0 \). This condition rules out Airy functions of the second kind (Bi\((z)\)) as solutions. Because of the symmetry of the potential, the solutions are alternately symmetric or antisymmetric. More precisely,
\[ \phi(p) = (\text{sgn} \ p)^n \text{Ai}(\kappa |p| - r_n), \] (18)
where \( \kappa \equiv (2D_1/(\hbar^2))^{1/3} \), and the \( r_n \)'s are the successive roots of Ai' (for \( n \) even), or of Ai (for \( n \) odd). The energy eigenvalues are
\[ E_n = -\left( \frac{k}{2} \hbar^2 D_1^2 \right)^{1/3} r_n. \] (19)
Note that \( r_n < 0 \), so \( E_n > 0 \).

Using the asymptotic expansion of the Airy function, we find that the roots are well approximated by
\[ r_n \approx -\left( \frac{3\pi}{4} \left( n + \frac{1}{2} \right) \right)^{2/3}, \quad n \in \{0\} \cup \mathbb{Z}^+ \] (20)
in the limit of large \( n \). This approximation reproduces the result of the WKB approximation above. This approximate formula is off by 8.7\% for \( n = 0 \), 0.77\% for \( n = 1 \), and 0.41\% for \( n = 2 \), and rapidly becomes more accurate for larger \( n \). Inserting Eq. (20) into Eq. (19) thus gives a very good approximate formula for the energies of the simple harmonic oscillator for \( \alpha = 1 \).
V. CONCLUSIONS

It would be useful to know the correct ground state of the one-dimensional infinite square well or harmonic oscillator for general $\alpha$, but this is a difficult problem. In Ref. \[15\], Bañuelos et al. needed a lengthy proof merely to show that the ground state solution for the infinite square well in the region $(-1,1)$ is concave on the interval $(-\frac{1}{\sqrt{2}}, +\frac{1}{\sqrt{2}})$.

Similar technical issues regarding nonlocality have arisen in the statistical mechanics community as well. For example, in Ref. \[16\], the authors claimed to analytically determine the mean first passage time for a Lévy flight with absorbing boundary conditions on the interval $[0, 1]$. They did so by imposing the standard absorbing boundary conditions for the probability density at $x = 0$ and $x = L$. However, a subsequent publication \[17\] pointed out that due to the nonlocal nature of the Lévy flight, the correct boundary condition is for the probability density to vanish for all $x \leq 0$, and for all $x \geq L$, rendering the analysis in Ref. \[16\] invalid.

Finally, one must also ask about possible physical realizations of the fractional Schrödinger equation. In Ref. \[12\], Zoia, Rosso, and Kardar constructed a lattice model whose continuum limit is described by fractional diffusion using symmetric Toeplitz matrices. A quantum representation of this model via a mesoscopic network of long range connections whose hopping amplitudes are described by the entries of these matrices may be a realization of the fractional Schrödinger equation. Further modification could lead to experimental tests of the problems we have discussed here.

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