Uniqueness of the fractional derivative definition

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For the Riesz fractional derivative besides the well known integral representation two new differential representations are presented, which emphasize the local aspects of a fractional derivative. The consequences for a valid solution of the fractional Schrödinger equation are discussed.

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I. INTRODUCTION

The concept of action-at-a-distance has dominated the interpretation of physical dynamic behavior in the early years of classical mechanics at the times of Kepler [1] and Newton [2]. In the second half of the 19th century the introduction of a field, first successfully applied in the electromagnetic theory of Maxwell [3], has led to a change of paradigm away from the previously accepted non-local view to an emphasis of local aspects of a given interaction. This development found its culmination in the case of gravitational interaction with Einstein’s geometric interpretation in terms of a space deformation [4].

On the other hand, the increasing success of quantum theory since the beginning of the 20th century may be interpreted as a renaissance of non-local concepts in physics and at the time present the interest in non-local field theories is steadily growing.

A non-relativistic description of quantum particles may be given using the Schrödinger wave equation. In this case, a new facet of non-locality may be introduced extending the standard local Laplace operator by its non-local fractional pendant. Fractional calculus introduces a new property, which only recently attracted attention on a broader basis.

\begin{table}[h!]
\centering
\begin{tabular}{|c|c|c|c|c|c|c|c|c|}
\hline
$N$ & $a_0$ & $a_{\pm 1}$ & $a_{\pm 2}$ & $a_{\pm 3}$ & $a_{\pm 4}$ & $a_{\pm 5}$ & $a_{\pm 6}$ & $a_{\pm 7}$ \\
\hline
1 & -2 & 1 & & & & & & \\
2 & -15/4 & 1/2 & 1/4 & & & & & \\
3 & -21/4 & 1/3 & 1/3 & & & & & \\
4 & -205/4 & 5/6 & 1/6 & & & & & \\
5 & -5269/5 & 17/5 & 1/5 & & & & & \\
6 & -88200/7 & 245/7 & 1/7 & & & & & \\
7 & -266681/7 & 720/7 & 2/7 & 2/7 & & & & \\
\hline
\end{tabular}
\caption{coefficients $a_n$ for a central difference approximation of the second derivative of the form $\sum_{n=-N}^{N} a_n f(x + n\xi)$, from [10] used in the definition of the generalized Riesz derivative $\alpha/2$.}
\end{table}

Let the one dimensional fractional stationary Schrödinger equation in scaled canonical form be defined as

$$-\Delta^{\alpha/2}\Psi(x) = (E - V(x))\Psi(x)$$

with the fractional Laplace-operator $\Delta^{\alpha/2}$. The definition of a fractional order derivative is not unique, several definitions e.g. the Riemann [11], Caputo [12], Riesz [13], Feller [14] coexist and are equally well suited for an extension of the standard derivative.

In order to preserve Hermiticity for the fractional extension of the Laplace-operator [10], we will explicitly consider the Riesz fractional derivative [13, 14]:

$$\Delta^{\alpha/2}f(x) \equiv \sum_{n=0}^{\infty} \partial_\alpha^n f(x)$$

$$= \Gamma(1 + \alpha) \sin(\pi\alpha/2) \times \int_0^\infty \frac{f(x + \xi) - 2f(x) + f(x - \xi)}{\xi^{\alpha+1}} d\xi$$

where the left superscript in $\sum_{n=0}^{\infty} \partial_\alpha^n f(x)$ emphasizes the fact, that the integral domain is the full space $\mathbb{R}$ and therefore explicitly denotes the non-local aspect of this definition.

Since there is an actual discussion about non-local aspects of a fractional derivative [10-23], in the following we will investigate the uniqueness of its definition. Within our discourse, we will present equivalent local representations of the Riesz derivative, which may be considered as a legitimation of e.g. piecewise solution of a fractional wave equation.
II. UNIQUENESS ON A GLOBAL SCALE - THE INTEGRAL REPRESENTATION

In order to investigate the uniqueness of a definition of a fractional derivative we will consider the Riesz derivative as an example. In this section, we will investigate a set of generalized integral representations.

We may determine the Riesz derivative as a specific symmetrized non-local generalization of the standard second order derivative\(^{15}\). We have

\[
\frac{\Gamma}{\eta^2} \partial^\alpha_x f(x) = \frac{\partial^2 f(x)}{\partial x^2} f(x) = 2\Gamma(\alpha - 1) \frac{\sin(\pi \alpha/2)}{\pi} \times \int_0^\infty \xi^{1-\alpha} f''(x + \xi) + f''(x - \xi) \quad \text{for} \quad \alpha > 1
\]

which indeed looks as a unique definition for the Riesz fractional derivative. The eigenfunctions of this operator are the trigonometric functions and the eigenvalues are given by:

\[
\frac{\Gamma}{\eta^2} \partial^\alpha_x \exp(ikx) = -|k|^\alpha \exp(ikx)
\]

\[
\frac{\Gamma}{\eta^2} \partial^\alpha_x \cos(kx) = -|k|^\alpha \cos(kx)
\]

\[
\frac{\Gamma}{\eta^2} \partial^\alpha_x \sin(kx) = -|k|^\alpha \sin(kx)
\]

Since \(\xi\) is nothing but a weighted sum of the simplest central difference approximation of the second derivative:

\[
f''(x) = \frac{f(x + \xi) - 2f(x) + f(x - \xi)}{\xi^2} + o(f^{(4)}(\xi))
\]

we may consider more sophisticated definitions of the Riesz derivative as a result of using higher accuracy approximations of the standard second order derivative, which are given as a finite series over \(2N + 1\) elements

\[
f''(x) = \frac{1}{\xi^2} \sum_{n=-N}^{N} a_n f(x + n\xi) + o(f^{(2N+2)}(\xi))
\]

with the properties, resulting from the requirement of a vanishing second derivative for a constant function and invariance under parity transformation \(\Pi(\pm \xi)\) with positive parity:

\[
\sum_{n=-N}^{N} a_n = 0, \quad a_{-n} = a_n
\]

In table I we have compiled the lowest representations of these finite series for \(N = 1, \ldots, 7\).

Therefore we may define the following generalization of the Riesz fractional derivative \(\not{\eta} \partial^\alpha_x\):

\[
\not{\eta} \partial^\alpha_x f(x) = \Gamma(1 + \alpha) \frac{\sin(\pi \alpha/2)}{\pi} \times \int_0^\infty \xi^{1-\alpha} \sum_{n=-N}^{N} a_n f(x + n\xi) \frac{1}{\xi^2}
\]

which at a first glance looks like a new family of fractional derivatives.

We will choose a pragmatic point of view and will investigate the eigenvalue spectrum of this set of operators. For that purpose, we use the following properties of the trigonometric functions\(^{24}\):

\[
\sin(z_1 \pm z_2) = \sin(z_1) \cos(z_2) \pm \cos(z_1) \sin(z_2)
\]

\[
\cos(z_1 \pm z_2) = \cos(z_1) \cos(z_2) \mp \sin(z_1) \sin(z_2)
\]

For \(f(x) = \cos(\nu x)\) it follows with\(^{12}\)

\[
\sum_{n=-N}^{N} a_n \cos(\nu x + n\xi)
\]

\[
= a_0 \cos(\nu x) + \sum_{n=1}^{N} a_n (\cos(\nu x - n\xi) + \cos(\nu x + n\xi))
\]

\[
= \cos(\nu x) (a_0 + 2 \sum_{n=1}^{N} a_n \cos(kn\xi))
\]

as a consequence, \(\cos(\nu x)\) is an eigenfunction of the generalized Riesz derivative operator \(\not{\eta} \partial^\alpha_x\). The same statement also holds for \(\sin(\nu x)\). It follows:

\[
\not{\eta} \partial^\alpha_x \exp(ik\nu x) = \kappa \exp(ik\nu x)
\]

\[
\not{\eta} \partial^\alpha_x \cos(k\nu x) = \kappa \cos(k\nu x)
\]

\[
\not{\eta} \partial^\alpha_x \sin(k\nu x) = \kappa \sin(k\nu x)
\]

with the eigenvalue spectrum \(\kappa\):

\[
\kappa = \Gamma(1 + \alpha) \frac{\sin(\pi \alpha/2)}{\pi} \times \int_0^\infty \xi^{1-\alpha} \left( a_0 + 2 \sum_{n=1}^{N} a_n \cos(kn\xi) \right)
\]

For \(n = 1\) we obtain the Riesz result \(\kappa = -|k|^\alpha\).

For \(n > 1\) since the integral covers the whole \(\mathbb{R}^+\), we may apply a coordinate transformation of the type \(\nu \xi = \xi\) to each term in the sum above. It then follows:

\[
\kappa = \Gamma(1 + \alpha) \frac{\sin(\pi \alpha/2)}{\pi} \times \int_0^\infty \xi^{1-\alpha} \left( a_0 + 2 \sum_{n=1}^{N} n^{\alpha} a_n \cos(k\xi) \right)
\]

\[
= \Gamma(1 + \alpha) \frac{\sin(\pi \alpha/2)}{\pi} \times \int_0^\infty \xi^{1-\alpha} \left( a_0 + 2 \sum_{n=1}^{N} n^{\alpha} a_n \cos(\xi) \right)
\]

\[
= |k|^\alpha \left( a_0 + \sum_{n=1}^{N} n^{\alpha} a_n \right), \quad 0 < \alpha < 2
\]
or in short hand notation:

$$\kappa = -\zeta_0(\alpha, N)|k|^\alpha$$  \hspace{1cm} (26)$$

Up to a scaling constant $\zeta_0(\alpha, N) = -(a_0 + \sum_{n=1}^{N} n^\alpha a_n)$ the eigenvalue spectrum is identical with the original Riesz derivative eigenvalue spectrum \cite{24} \cite{25} and may be absorbed by proper normalization of the generalized Riesz derivative definition.

Therefore all generalized derivative definitions of type \cite{13}, which obey conditions \cite{12} are equivalent and lead to same results. In that sense, the Riesz definition of a second order fractional derivative is indeed unique and emphasizes the non-local aspects of a fractional derivative.

It should be emphasized, that alternative realizations of the fractional Riesz derivative in terms of e.g. a central differences representation of Grünwald-Letnikov type are equivalent to the above integral representation in their non-local behavior \cite{26} \cite{28}.

In the next section we will investigate the differential representation of the Riesz derivative and will demonstrate in a similar way as in the case of the integral representations that different approaches lead to the same result.

III. UNIQUENESS ON A LOCAL SCALE - THE DIFFERENTIAL REPRESENTATION

Differential representations of the Riemann and Caputo fractional derivative in terms of a series expansion of integer derivatives are commonly known \cite{6} \cite{9} \cite{23} \cite{30}. This approach emphasizes the local aspects of a fractional derivative. A corresponding series expansion for the Riesz derivative would lead to a local representation of the same fractional derivative.

Indeed there are several strategies to derive a differential representation of the Riesz derivative. Let us begin with the fractional extension of the binomial series \cite{24} \cite{23}:

$$\partial_x^\alpha = \lim_{\omega \rightarrow 0} (\partial_x + \omega)^\alpha = \lim_{\omega \rightarrow 0} \sum_{j=0}^{\infty} \binom{\alpha}{j} \omega^{\alpha-j} \partial_x^j \hspace{1cm} \alpha \in \mathbb{R}$$  \hspace{1cm} (27)$$

where $\omega$ is an arbitrary real number.

Motivated by the correspondence

$$\lim_{\alpha \rightarrow 2|\omega|} \partial_x^\alpha = \partial_x^2$$  \hspace{1cm} (28)$$

which holds for the Riesz derivative, we extend the above binomial series to

$$\triangle \partial_x^\alpha = \lim_{\omega \rightarrow 0} (\partial_x^2 + \omega^2)^{\alpha/2} = \lim_{\omega \rightarrow 0} \sum_{j=0}^{\infty} \binom{\alpha/2}{j} (\omega^2)^{\alpha/2-j} \partial_x^{2j}$$  \hspace{1cm} (29)$$

$$= \lim_{\omega \rightarrow 0} |\omega|^\alpha \sum_{j=0}^{\infty} \binom{\alpha/2}{j} |\omega|^{-2j} \partial_x^{2j} \hspace{1cm} \alpha \in \mathbb{R}$$  \hspace{1cm} (30)$$

where the superscript $\triangle$ emphasizes the differential representation of an hitherto integral representation of a fractional derivative operator $\partial_x^\alpha$.

Applying this operator to the exponential function leads to:

$$\triangle \partial_x^\alpha \exp(kx) = \lim_{\omega \rightarrow 0} \sum_{j=0}^{\infty} \binom{\alpha/2}{j} (\omega^2)^{\alpha/2-j} k^{2j} \exp(kx)$$  \hspace{1cm} (32)$$

$$= \lim_{\omega \rightarrow 0} (k^2 + \omega^2)^{\alpha/2} \exp(kx)$$  \hspace{1cm} (33)$$

$$= |k|^{\alpha} \exp(kx) \hspace{1cm} \alpha \in \mathbb{R}$$  \hspace{1cm} (34)$$

Consequently we interpret this operator as the hyperbolic Riesz derivative, since it works for $k \in \mathbb{R}$, while the original Riesz derivative in its integral form is divergent for $\exp(kx)$ but converges for $\exp(ikx)$.

Therefore in an heuristic approach we obtain as a differential representation of the Riesz derivative:

$$\triangle \partial_x^\alpha = \lim_{\omega \rightarrow 0} |\omega|^\alpha \sum_{j=0}^{\infty} \binom{\alpha/2}{j} |\omega|^{-2j} (-1)^j \partial_x^{2j}$$  \hspace{1cm} (35)$$

$$\triangle \partial_x^\alpha = \lim_{\omega \rightarrow 0} |\omega|^\alpha \sum_{j=0}^{\infty} \binom{\alpha/2}{j} |\omega|^{-2j} (i\partial_x)^{2j}$$  \hspace{1cm} (36)$$

which we call a valid realization of the differential form of the Riesz fractional derivative.

Indeed it follows in accordance with \cite{24} \cite{25}:

$$\triangle \partial_x^\alpha \exp(ikx) = -|k|^\alpha \exp(ikx)$$  \hspace{1cm} (37)$$

$$\triangle \partial_x^\alpha \cos(kx) = -|k|^\alpha \cos(kx)$$  \hspace{1cm} (38)$$

$$\triangle \partial_x^\alpha \sin(kx) = -|k|^\alpha \sin(kx) \hspace{1cm} \alpha \in \mathbb{R}$$  \hspace{1cm} (39)$$

Since we have realized the differential form of the Riesz derivative as the limit of a series we will answer the question if other series may yield the same result.

As a demonstration, we use the fractional extension of the Leibniz product rule \cite{31} \cite{32}:

$$\partial_x^\alpha (u(x)v(x)) = \sum_{j=0}^{\infty} \binom{\alpha}{j} (\partial_x^{\alpha-j} u(x))(\partial_x^j v(x))$$  \hspace{1cm} (40)$$

and rewrite the analytic function $f(x)$ as

$$f(x) = \lim_{\omega \rightarrow 0} \cos(\omega x) f(x)$$  \hspace{1cm} (41)$$

With \cite{31} follows:

$$\triangle \partial_x^{\alpha-j} \lim_{\omega \rightarrow 0} \cos(\omega x)$$  \hspace{1cm} (42)$$

$$= \lim_{\omega \rightarrow 0} (\partial_x^{-j} \partial_x^\alpha) \cos(\omega x)$$  \hspace{1cm} (43)$$

$$= \lim_{\omega \rightarrow 0} -|\omega|^\alpha \partial_x^{-j} \cos(\omega x)$$  \hspace{1cm} (44)$$

$$= \lim_{\omega \rightarrow 0} -|\omega|^\alpha \omega^{-j} \cos(\omega x - \frac{\pi}{2} j)$$  \hspace{1cm} (45)$$

$$= \lim_{\omega \rightarrow 0} -|\omega|^\alpha \omega^{-j} \begin{cases} 0 & j \text{ odd} \\ (-1)^{j/2} & j \text{ even} \end{cases}$$  \hspace{1cm} (46)$$
Using the Leibniz product rule we obtain:

\[ \triangle \partial_x^\alpha = \lim_{\omega \to 0} \sum_{j=0}^{\infty} \left( \frac{\alpha}{j} \right) (\partial_x^{\alpha-j} \cos(\omega x)) \partial_x^j \]

\[ = -\lim_{\omega \to 0} |\omega|^\alpha \sum_{j=0}^{\infty} \left( \frac{\alpha}{2j} \right) \omega^{-2j} (-1)^j \partial_x^{2j} \]

\[ = -\lim_{\omega \to 0} |\omega|^\alpha 2F_1(\frac{1}{2} - \frac{\alpha}{2}, -\frac{\alpha}{2}; 1; -\frac{k^2}{\omega^2}) \]  

(48)

Let apply this operator to the exponential function:

\[ \triangle \partial_x^\alpha \exp(kx) \]

\[ = -\lim_{\omega \to 0} |\omega|^\alpha 2F_1(\frac{1}{2} - \frac{\alpha}{2}, -\frac{\alpha}{2}; 1; -\frac{k^2}{\omega^2}) \exp(kx) \]

\[ = -|k|^\alpha \cos(\alpha \pi/2) \exp(kx) \]

(50)

where we have used (15.3.7) and (15.1.8) from [22].

Once again, we may consider this operator as an alternative realization of a hyperbolic Riesz derivative, since it works for \( k \in \mathbb{R} \), while the original Riesz derivative in its integral form is divergent for \( \exp(kx) \) but converges for \( \exp(ikx) \).

Therefore we define a differential representation of the Riesz derivative heuristically:

\[ \triangle \partial_x^\alpha = \lim_{\omega \to 0} |\omega|^\alpha \sum_{j=0}^{\infty} \left( \frac{\alpha}{2j} \right) \omega^{-2j} \partial_x^{2j} \]

(51)

\[ = -\frac{1}{\cos(\alpha \pi/2)} \lim_{\omega \to 0} |\omega|^\alpha 2F_1(\frac{1}{2} - \frac{\alpha}{2}, -\frac{\alpha}{2}; 1; -\frac{1}{\omega^2}) \partial_x^{2j} \]

(52)

with the same eigenfunctions and eigenvalue spectrum [37]-[39].

Hence we have demonstrated, that indeed there exist different differential representations, which in the limit \( \omega \to 0 \) lead to the same eigenvalue spectrum.

IV. MANIFEST COVARIANT LOCAL REPRESENTATION OF THE RIESZ DERIVATIVE ON \( \mathbb{R}^N \)

A straightforward extension of e.g. [52] to the N-dimensional case is given by

\[ \triangle \triangle^{\alpha/2}_N = -\frac{1}{\cos(\alpha \pi/2)} \lim_{\omega \to 0} |\omega|^\alpha 2F_1(\frac{1}{2} - \frac{\alpha}{2}, -\frac{\alpha}{2}; \omega; \triangle) \]

(53)

with the N-dimensional Laplace-operator \( \triangle \) in cartesian coordinates on \( \mathbb{R}^N \)

\[ \triangle = \sum_{n=1}^{N} \partial_n^2 \quad N \in \mathbb{N} \]

(54)

The eigenfunctions and the eigenvalue spectrum of this differential representation of the N-dimensional Riesz derivative is then given by:

\[ \triangle \triangle^{\alpha/2}_N \prod_{n=1}^{N} \exp(ik_n x_n) = -\frac{N}{\sum_{n=1}^{N} k_n^{\alpha/2}} \prod_{n=1}^{N} \exp(ik_n x_n) \]

(55)

which coincides with the standard result using the standard integral representation.

In a similar approach we may extend (50) to the N-dimensional case:

\[ \triangle \triangle^{\alpha/2}_N \lim_{\omega \to 0} |\omega|^\alpha \sum_{j=0}^{\infty} \left( \frac{\alpha}{2j} \right) |\omega|^{-2j} (-1)^j \triangle^j \]

(56)

Since the Laplace-operator may be derived for any set of coordinates, where the metric tensor \( g_{ij} \) is known [4] via:

\[ \triangle = g^{ij} \nabla_i \nabla_j \quad i, j = 1, ..., N \]

(57)

\[ = \frac{1}{\sqrt{g}} \partial_i g^{ij} \sqrt{g} \partial_j \]

(58)

\[ = g^{ij} (\partial_i \partial_j - \{ k \}_{ij}) \]

(59)

where \( \nabla_i \) denotes the Riemann covariant derivative, \( g \) is the determinant of the metric tensor, \( g = \det g_{ij} \) and \( \{ k \}_{ij} \) is the Christoffel symbol. [53] and [50] may be considered as two optional candidates for a differential representation of a valid covariant realization of the Riesz fractional derivative on the Riemannian space.

V. CONCLUSION

With [53] and [50] we have presented two different realizations of a differential representation of the Riesz derivative as a limiting case of two different series expansions in terms of integer derivatives.

At least in the case of the trigonometric functions \( \sin(kx) \) and \( \cos(kx) \) and therefore for every Fourier series these series are convergent and valid for all \( \alpha \in \mathbb{R} \) and thus are more robust than their integral counterparts, where the range of allowed \( \alpha \) values is restricted to \( 0 < \alpha < 2 \).

It is important to mention, that these representations are realized as series in terms of standard derivatives and therefore determine a local version of the fractional derivative, since information is required only within an \( \epsilon \)-region around \( x \). The use of a fractional derivative does not automatically imply non-locality.

As a consequence, using the differential representations of the Riesz derivative, it seems a valid procedure to generate piecewise steady solutions of a Riesz type fractional Schrödinger equation even though in a way this contradicts Feynman’s view of a path integral formulation of quantum mechanics.
Consequently while in standard quantum mechanics Schrödinger’s wave equation as a local view and Feynman’s path integral approach as a non-local view lead to equivalent results, in fractional quantum mechanics this equivalence obviously is lost and leads to different results \[10-23\]. Hence using the Riesz fractional derivative given in terms of either the integral or the differential representation indeed makes a difference in e.g. fractional wave equations. Emphasizing fundamentally different aspects of a local or non-local approach to physical problems the use of the Riesz fractional derivative in either form revives the discussion of concepts like action-at-a-distance.

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