DISCUSSION SURVEY

EXPERIMENTAL IMPLICATIONS OF BOCHNER-LEVY-RIESZ DIFFUSION

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Abstract

Fractional Bochner-Levy-Riesz diffusion arises from ordinary diffusion by replacing the Laplacean with a noninteger power of itself. Bochner-Levy-Riesz diffusion as a mathematical model leads to nonlocal boundary value problems. As a model for physical transport processes it seems to predict phenomena that have yet to be observed in experiment.

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1. Introduction

Applications of fractional differentiation in physics [10] have become widespread (see the reviews in [10, 12, 28, 29] and references therein). Despite the wide dissemination of fractional models some basic questions and fundamental problems persist [12].

My objective in this note is to discuss the applicability of fractional Bochner-Levy diffusion and fractional Riesz potentials as a mathematical model for physical phenomena. A lively scientific debate is presently concerned with boundary value problems for fractional Laplaceans and their relevance for experiment as witnessed by the special session devoted to nonlocal boundary value problems at the recent International Conference on Fractional Differentiation and Its Applications in Catania, June 23-25,

2014. In view of this ongoing debate it seems timely to contribute to the discussion by exploring some thoughts of the present author concerning implications of nonlocality for experiments [12, Section 2.3.2,p.48], that were pointed out again at the conference. Originally, fractional derivatives and Riesz potentials were introduced as a convenient calculational tool (see e.g. [19, 22, 23]). Recently, however, fractional differential equations have often been proposed as "generalizations" of more or less fundamental equations of physics and engineering. Examples range from Schrödinger [17] and advection-dispersion equations [27, 3, 4] to viscoelasticity [1], suspension bridges [24] or loudspeaker coils [25]. Many generalizations remain formal in the sense that their rigorous relation to established theories is unknown and their limits of validity have not been worked out.

Deep and fundamental principles of physics suggest that mathematical models of physical phenomena must always be formulated in terms of spatial derivatives of integer order (see [6]). Electrodynamics, hydrodynamics, mechanics and quantum theory do not feature (spatial or temporal) fractional derivatives. It is therefore not impossible that formal fractionalization of fundamental equations might produce interesting mathematical models that predict phenomena not observed in experiment.

Given the large number of differential equations that have already been fractionalized this short note will restrict attention to a specific example. Let me choose fractional Bochner-Levy diffusion as this specific example, because it has been a focus of attention both in mathematics and physics. One can fractionalize the ordinary diffusion equation in several ways. Replacing the Laplacean with a fractional derivative is one possibility. It is called called Bochner-Levy or Riesz fractional diffusion [18, 22, 2]. Another possibility, called Montroll-Weiss fractional diffusion, is to introduce a fractional time derivative [21, 26, 7, 13, 9, 11, 12]. Mathematically it is equivalent to the the theory of continuous time random walks [20] as first observed in [8].

2. Mathematical Model

Let $\Delta = \sum_{i=1}^{d} \partial^2/\partial x_i^2$ denote the d-dimensional Laplace operator in cartesian coordinates. Numerous authors postulate a fractional diffusion equation such as

$$\frac{\partial u}{\partial t} = -(-\Delta)^{\alpha/2} u(x,t), \qquad x \in \mathbb{B} \subseteq \mathbb{R}^d, \ \ t \geq 0, \qquad (2.1)$$

with $0 < \alpha \leq 2$ and initial condition

$$u(x,0) = h(x), \qquad x \in \mathbb{B} \subseteq \mathbb{R}^d \qquad (2.2)$$

for a function $u : \mathbb{R}^d \to \mathbb{R}$ as a mathematical model for various physical phenomena (see [10, 15, 14, 28, 29] for examples). For $\alpha = 2$ this becomes the Cauchy problem for the ordinary diffusion equation whose applicability as a mathematical model for physical phenomena has been validated with innumerable experiments. For $0 < \alpha < 2$ however experimental evidence remains narrowly bounded in space and time scales. Moreover, theoretical considerations cast fundamental doubts on the applicability of this case to natural phenomena.

For $\mathbb{B} = \mathbb{R}^d$ the fractional Laplace operator $(-\Delta)^{\alpha/2}$ in eq. (2.1) may be defined (in the sense of Riesz [23]) as

$$\mathcal{F}\left\{(-\Delta)^{\alpha/2} f(x)\right\}(k) = |k|^\alpha \mathcal{F}\left\{f(x)\right\}(k), \qquad (2.3)$$

where $\mathcal{F}\left\{f(x)\right\}(k)$ denotes the Fourier transform of $f(x)$. A core domain suitable for various extensions are functions $f \in \mathcal{S}(\mathbb{R}^d)$ from the Schwartz space of smooth functions decreasing rapidly at infinity.

The implicit idealizing assumption underlying the choice of an un-bounded domain $\mathbb{B} = \mathbb{R}^d$ in eq. (2.1) is that the boundary is sufficiently far away so that its effects on the observations are negligible. However, experiments are normally performed inside a bounded laboratory containing a bounded apparatus that occupies a bounded domain $\mathbb{B} \subset \mathbb{R}^d$ of space. Thus, practical applications require to consider nonlocal boundary value problems on bounded domains $\mathbb{B} \subset \mathbb{R}^d$.

Every experiment assumes that the experimental conditions in the region $\mathbb{R}^d \backslash \mathbb{B}$ surrounding the region $\mathbb{B}$ containing the sample can be controlled and reproduced to any desired degree of accuracy. In the mathematical model this is represented by assuming given boundary data $g : \mathbb{R}^d \backslash \mathbb{B} \to \mathbb{R}$ for the unknown $u(x, t)$ such that

$$u(x, t) = g(x), \qquad x \in \mathbb{R}^d \backslash \mathbb{B} \qquad (2.4)$$

for all times $t \geq 0$. The Riesz operator $(-\Delta)^{\alpha/2}$ may then be be understood as a Dirichlet form on the space $L^2(\mathbb{B}, \mu)$ over the bounded set $\mathbb{B}$ equipped with the canonical Borel σ-algebra and a σ-finite measure μ, [5].

3. Discussion

3.1. (Non-)locality and (in-)finite propagation speed

It is the primary objective of this note to contribute to the current debate by discussing fundamental differences between the cases $\alpha = 2$ and $0 < \alpha < 2$ in eq. (2.1) for applications to experiment. The decisive difference between the cases $\alpha = 2$ and $0 < \alpha < 2$ is the locality of the Laplacean $-\Delta$ for $\alpha = 2$ in contrast with the nonlocality of the fractional Laplacean $(-\Delta)^{\alpha/2}$ for $0 < \alpha < 2$.

Before discussing the (non-)locality of $(-\Delta)^{\alpha/2}$ it seems important to distinguish it from another nonlocality appearing in eq. (2.1). It is sometimes argued that also the case $\alpha = 2$ shows nonlocality in the sense that a localized initial condition such as $u(x,0) = h(x) = \delta(x - x_0)$, vanishing everywhere except at x_0 for $t = 0$, spreads out instantaneously to all x such that $u(x,t) \neq 0$ for all x for $t > 0$. This initially infinite "speed of propagation" violates relativistic locality. While this is true for all $0 < \alpha \leq 2$, it concerns the operator $\partial/\partial t + (-\Delta)^{\alpha/2}$ and occurs only at $t = 0$, the initial instant. For $\alpha = 2$ the operator Δ is local and also $\partial/\partial t + (-\Delta)$ is perfectly local for all $t > 0$. While an infinite propagation speed occurs also for $0 < \alpha < 2$ another violation of locality occurs in this case. This has more dramatic implications for experiment, as will now be discussed.

3.2. Probabilistic interpretation

The fundamental difference between the cases $\alpha = 2$ and $0 < \alpha < 2$ can be understood from the deep and well known relation between the diffusion equation (2.1) and the theory of stochastic processes. The probabilistic interpretation of $u(x)$ is given in terms of families of stochastic processes $(X_t)_{t \geq 0}$ indexed by their starting point $X_0 = x \in \mathbb{B}$ through the formula (for a sphere $\mathbb{B} = \mathbb{B}(z, R) = \{x \in \mathbb{R}^d : |x - z| < R\}$ of radius R around z for simplicity)

$$u(x) = \langle u(X_{T^e(\mathbb{R}^d \setminus \mathbb{B}(z,R))}) \rangle_x, \tag{3.5}$$

where $T^e(\mathbb{R}^d \setminus \mathbb{B}(z, R))$ denotes the first exit time of a path starting at $X_0 = x \in \mathbb{B}(z, R)$ and hitting the set $\mathbb{R}^d \setminus \mathbb{B}(z, R)$ for the first time at $t = T^e(\mathbb{R}^d \setminus \mathbb{B}(z, R))$. The brackets $\langle Y \rangle_x$ denote the expectation value of a random variable Y evaluated for the process $(X_t)_{t \geq 0}$ starting from x at $t = 0$.

For $\alpha = 2$ the family of stochastic processes has almost surely continuous paths. Because of this, a path starting from $x \in \mathbb{B}(z, R)$ at $t = 0$ will exit from $\mathbb{B}(z, R)$ when hitting $\partial \mathbb{B}(z, R) = \{x \in \mathbb{R}^d : |x - z| = R\}$ for the first time.

For $0 < \alpha < 2$ on the other hand the families of stochastic processes have almost surely discontinuous paths that can jump over the boundary $\partial \mathbb{B}(z, R)$. As a result the first exit occurs not at the boundary but at some point $X_{T^e(\mathbb{R}^d \setminus \mathbb{B}(z,R))}$ deep in the exterior region $\mathbb{R}^d \setminus \mathbb{B}(z, R)$.

In applications to particle diffusion the unknown $u(x,t)$ is often the concentration of atomic, molecular or tracer particles and fractional generalizations of Fick's law have been postulated [4, 27, 3]. Note, however, that the probabilistic interpretation is frequently not physical even for $\alpha = 2$. There are at least two possible reasons: Firstly, the underlying physical dynamics may not be stochastic. Secondly, fundamental laws of probability

theory may be violated as for the case of heat diffusion where $u(x,t)$ is the temperature field. In such cases the random "paths" are fictitious as are the "particles" and their "trajectories" in the sense that they cannot be observed directly in an experiment.

Whether or not a probabilistic interpretation applies, the discontinuity of the trajectories in the probabilistic interpretation leads to experimental difficulties. This can be seen from considering the stationary states of (2.1),(2.2) and (2.4).

3.3. Stationary solutions

To explore the physical consequences of the initial and boundary value problem (2.1),(2.2) and (2.4) it is useful to start with stationary solutions, i.e. solutions of the form

$$u(x,t) = u(x). \tag{3.6}$$

The fractional diffusion equation then reduces to the fractional Riesz-Dirichlet problem

$$(-\Delta)^{\alpha/2} u(x) = 0, \qquad x \in \mathbb{B} \tag{3.7a}$$

$$u(x) = g(x), \qquad x \in \mathbb{R}^d \setminus \mathbb{B} \tag{3.7b}$$

for suitable boundary data $g(x)$ such that

$$\int_{\mathbb{R}^d \setminus \mathbb{B}} \frac{|g(x)|}{1 + |x|^{d+\alpha}} \, \mathrm{d}^d x < \infty \tag{3.8}$$

holds.

The solution of the fractional Riesz-Dirichlet problem for the case of a sphere $\mathbb{B} = \mathbb{B}(z, R) = \{x \in \mathbb{R}^d : |x - z| < R\}$ of radius R centered at $z \in \mathbb{R}^d$ is the fractional Poisson integral [16]

$$u(x) = \frac{\Gamma\left(\frac{d}{2}\right) \sin\left(\frac{\pi\alpha}{2}\right)}{\pi^{\frac{d}{2}+1}} \int_{\mathbb{R}^d \setminus \mathbb{B}(z,R)} \frac{\left|R^2 - |x - z|^2\right|^{\frac{\alpha}{2}}}{|R^2 - |y - z|^2|^{\frac{\alpha}{2}} \, |x - y|^d} g(y) \mathrm{d}^d y \tag{3.9}$$

for $x \in \mathbb{B}(z, R)$. For $\alpha \to 2$ the solution reduces to the conventional Poisson integral

$$u(x) = \frac{\Gamma(d/2)}{2R\pi^{d/2}} \int_{\partial\mathbb{B}(z,R)} \frac{R^2 - |x - z|^2}{|x - y|^d} g(y) \mathrm{d}^{d-1} y \tag{3.10}$$

for $x \in \mathbb{B}(z, R)$ and $u(x) = g(x)$ for $x \in \partial\mathbb{B}(z, R)$.

Although the fractional Poisson formula eq. (3.9) has been known for nearly 70 years [22] its crucial difference to (3.10) seems to have escaped the attention of those scientists, who propose eq. (2.1) or its variants as a mathematical model for physical phenomena. Perhaps this is due to

the fact that many workers assume explicitly or implicitly "absorbing" or "killing" boundaries $g = 0$ for all $x \in \mathbb{R}^d \setminus \mathbb{B}(z, R)$. Physically this means that there are no atoms, molecules or tracer particles outside the spherical container $\mathbb{B}(z, R)$. Any particle that jumps out of $\mathbb{B}(z, R)$ is considered to be instantaneously removed from the experiment. The environment surrounding the experimental apparatus has to be kept absolutely clean at all times for these boundary conditions to apply. Under these experimental conditions both equations, eq. (3.9) as well as eq. (3.10), agree and both predict

$$u(x) = 0 \tag{3.11}$$

for all $x \in \mathbb{R}^d$ and all $0 < \alpha \leq 2$.

Consider next the case when there exist regions where the atomic, molecular or tracer particles are not instantaneously removed. For simplicity let there exist several small nonoverlapping spherical containers $\mathbb{B}(z_i, R_i)$ with $i = 1, ..., n$, $\mathbb{B}(z_i, R_i) \cap \mathbb{B}(z_j, R_j) = \emptyset$ for all $i \neq j$ and $\mathbb{B}(z_i, R_i) \cap \mathbb{B}(z, R) = \emptyset$ for all i in which particles are kept (e.g. for replenishment). This means that in these containers $g(x) \neq 0$ and particles jumping out of the sample region $\mathbb{B}(z, R)$ may land in one of these containers. They are not removed until the container is filled and a maximum concentration is reached. Let $u_i \in \mathbb{R}$ denote the maximal concentration in each container. Assume that

$$g(x) = \sum_{i=1}^{n} R_i^{-d} \phi_i \left(\frac{x - z_i}{R_i} \right) \tag{3.12a}$$

with

$$\phi_i(x) = \begin{cases} u_i \exp\left(-\frac{1}{1-|x|^2}\right) & \text{for } x \in \mathbb{B}(0, 1) \\ 0 & \text{otherwise} \end{cases} \tag{3.12b}$$

describes the concentration field in the region $\mathbb{R} \setminus \mathbb{B}(z, R)$ outside the sample. Other functions than $\phi_i(x)$ with $\operatorname{supp} \phi_i \subset \mathbb{B}(z_j, R_j)$ are possible. Assume also that $R_i \ll R$ for all i, so that in particular also $\operatorname{supp} g \cap \partial \mathbb{B}(z, R) = \emptyset$ holds.

For $\alpha = 2$ eq. (3.10) shows that the solution $u(x) = 0$ remains unaffected by the containers $\mathbb{B}(z_i, R_i)$ and their content. For $0 < \alpha < 2$ on the other hand the solution changes and becomes nonzero. It is approximately

$$u(x) \approx \frac{\Gamma\left(\frac{d}{2}\right) \sin\left(\frac{\pi \alpha}{2}\right)}{\pi^{\frac{d}{2}+1}} \sum_{i=1}^{n} \frac{u_i \left|R^2 - |x - z|^2\right|^{\frac{\alpha}{2}}}{\left|R^2 - |z_i - z|^2\right|^{\frac{\alpha}{2}} |x - z_i|^d} \neq 0 \tag{3.13}$$

for $x \in \mathbb{B}(z, R)$. This result implies that for $0 < \alpha < 2$ the stationary solution inside the sample region $\mathbb{B}(z, R)$ depends on the location and content of all other containers $\mathbb{B}(z_i, R_i)$ in the laboratory. The sample in $\mathbb{B}(z, R)$

cannot be shielded or isolated from other samples in the laboratory. It should be easy to verify or falsify this prediction in an experiment.

4. Conclusion

Fractional Bochner-Levy-Riesz diffusion represents an interesting mathematical generalization. It remains to be seen, however, whether and in which approximation fractional spatial derivatives can arise phenomenologically in mathematical models of an underlying physical reality that obeys spatial locality. If such an approximation should exist for physical particle transport processes, such that physical particle trajectories can be identified with the mathematical paths of a Levy process, then it seems to be an open problem how to understand the nonlocal dependence of stationary states in these systems on the location of, and particle concentration in distant and remote containers. It will also be interesting to understand whether and in which sense the experiments are reproducible and how an experimental apparatus can be shielded or isolated from the environment. Without experimental evidence for the mathematical predictions of fractional potential theory it seems difficult to reconcile nonlocality in space (i.e. the case $0 < \alpha < 2$) with theory and experiment.

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