SPACE-TIME FRACTIONAL DIFFUSION ON BOUNDED DOMAINS

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ABSTRACT. Fractional diffusion equations replace the integer-order derivatives in space and time by their fractional-order analogues. They are used in physics to model anomalous diffusion. This paper develops strong solutions of space-time fractional diffusion equations on bounded domains, as well as probabilistic representations of these solutions, which are useful for particle tracking codes.

1. Introduction

The traditional diffusion equation $\partial_t u = \Delta u$ describes a cloud of spreading particles at the macroscopic level. The point source solution is a Gaussian probability density that predicts the relative particle concentration. Brownian motion provides a microscopic picture, describing the paths of individual particles. A Brownian motion, killed or stopped upon leaving a domain, can be used to solve Dirichlet boundary value problems for the heat equation, as well as some elliptic equations [4][11]. The space-time fractional diffusion equation $\partial_t^\beta u = \Delta^{\alpha/2} u$ with $0 < \beta < 1$ and $0 < \alpha < 2$ models anomalous diffusion [19]. The fractional derivative in time can be used to describe particle sticking and trapping phenomena. The fractional space derivative models long particle jumps. The combined effect produces a concentration profile with a sharper peak, and heavier tails. This paper studies strong solutions, and probabilistic representations of solutions, for the space-time diffusion equation on bounded domains. Our main result is Theorem 5.1. Strong solutions are obtained by separation of variables, combining the Mittag-Leffler solution to the time-fractional problem with an eigenfunction expansion of the fractional Laplacian on bounded domains. The probabilistic representation of solutions involves an inverse stable subordinator time change, resulting in a non-Markovian process. Fractional diffusion equations are becoming popular in many areas of application [15][23]. In these applications, it is often important to consider boundary value problems. Hence it is useful to develop solutions for space-time fractional diffusion equations on bounded domains with Dirichlet boundary conditions.

Key words and phrases. Fractional derivative; anomalous diffusion; probabilistic representation, strong solution; Cauchy problem; bounded domain.

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2. RANDOM WALKS AND STABLE PROCESSES

A random walk $S_t = Y_1 + \cdots + Y_{[t]}$, a sum of independent and identically distributed $\mathbb{R}^d$-valued random vectors, is commonly used to model diffusion in statistical physics. Here $[t]$ denotes the largest integer not exceeding $t$, and $S_n$ represents the location of a random particle at time $n$. Suppose the distribution of $Y$ is spherically symmetric. If $\sigma^2 := \mathbb{E}[|Y_1|^2]$ is finite and $\mathbb{E}[Y_1] = 0$, Donsker’s invariance principle implies that as $\lambda \to \infty$, the random process $\{\lambda^{-1/2}S_M, t \geq 0\}$ converges weakly in the Skorohod space to a Brownian motion $\{B_t, t \geq 0\}$ with $\mathbb{E}[B_t^2] = \sigma^2$. If the step random variable $Y_1$ is spherically symmetric, and $\mathbb{P}(|Y_1| > x) \sim Cx^{-\alpha}$ as $x \to \infty$ for some $0 < \alpha < 2$ and $C > 0$, then $\mathbb{E}[|Y_1|^2]$ is infinite, and the extended central limit theorem tells us that $\{\lambda^{-1/\alpha}S_M, t \geq 0\}$ converges weakly to a rotationally symmetric $\alpha$-stable Lévy motion $\{A_t, t \geq 0\}$ with

$$\mathbb{E}[e^{i\xi A_t}] = e^{-C_0|\xi|^\alpha t} \quad \text{for every } \xi \in \mathbb{R}^d \text{ and } t \geq 0,$$

where the constant $C_0$ depends only on $C$ and the dimension $d$, see [18]. A simple rescaling in space yields a standard stable process with $C_0 = 0$. Since $\{\lambda^{1/\alpha}A_t, t \geq 0\}$ has the same distribution as $\{A_M, t \geq 0\}$, stable Lévy motion represents a model for anomalous super-diffusion, where particles spread faster than a Brownian motion [17].

If we impose a random waiting time $T_n$ before the $n$th random walk jump, then the position of the particle at time $T_n = J_1 + \cdots + J_n$ is given by $S_n$. The number of jumps by time $t > 0$ is $N_t = \max\{n : T_n \leq t\}$, so the position of the particle at time $t > 0$ is $S_{N_t}$, a subordinated process. If $\mathbb{P}(J_n > t) \sim Ct^{-\beta}$ as $t \to \infty$ for some $0 < \beta < 1$, then the scaling limit of $c^{-1/\beta}\tau_{[d]} \Rightarrow Z_t$ as $c \to \infty$ is a strictly increasing stable Lévy motion with index $\beta$, sometimes called a stable subordinator. The jump times $T_n$ and the number of jumps $N_t$ are inverses: $\{N_t \geq n\} = \{T_n \leq t\}$. [20] Theorem 3.2 shows that $\{c^{-\beta/\alpha}T_{[d]}, t \geq 0\}$ converges weakly to the process $\{E_t, t \geq 0\}$, where $E_t = \inf\{x : Z_x > t\}$. In other words, the scaling limits are also inverses: $\{E_t \leq x\} = \{Z_x \geq t\}$. Now $N_{ct} \approx c^\beta E_t$, and [20] Theorem 4.2 shows that the scaling limit of the particle location $\{c^{-\beta/\alpha}S_{N_{ct}}, t \geq 0\}$ is $\{A_{E_t}, t \geq 0\}$, a symmetric stable Lévy motion time-changed by an inverse stable subordinator.

The random variable $Z_t$ has a smooth density. For properly scaled waiting times, the density of the standard stable subordinator $Z_t$ has Laplace transform $\mathbb{E}[e^{-\eta Z_t}] = e^{-t\eta^\beta}$ for any $\eta, t > 0$, and $Z_t$ is identically distributed with $t^{1/\beta} Z_1$. Writing $g_\beta(u)$ for the density of $Z_1$, it follows that $Z_s$ has density $s^{-1/\beta}g_\beta(s^{-1/\beta} u)$ for any $s > 0$. Using the inverse relation $\mathbb{P}(E_t \leq s) = \mathbb{P}(Z_s \geq t)$ and taking derivatives, it follows that $E_t$ has the density

$$f_t(s) = \frac{d}{ds} \mathbb{P}(Z_s \geq t) = t^{\beta - 1}s^{-1-1/\beta}g_\beta(ts^{-1/\beta}).$$

For more details, see [19, 20].
3. FRACTIONAL CALCULUS

The Caputo fractional derivative of order $0 < \beta < 1$, defined by

\[
\frac{\partial^{\beta} f(t)}{\partial t^{\beta}} = \frac{1}{\Gamma(1-\beta)} \int_{0}^{t} \frac{\partial f(r)}{\partial r} (t-r)^{\beta-1} dr,
\]

was invented to properly handle initial values \[9, 13\]. Its Laplace transform (LT) $s^{\beta} \tilde{f}(s) - s^{\beta-1} f(0)$ incorporates the initial value in the same way as the first derivative. Here $\tilde{f}(s) = \int_{0}^{\infty} e^{-st} f(t) dt$ is the usual Laplace transform. The Caputo derivative has been widely used to solve ordinary differential equations that involve a fractional time derivative \[15, 24\]. In particular, it is well known that the Caputo derivative has a continuous spectrum, with eigenfunctions given in terms of the Mittag-Leffler function

\[
E_{\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(1 + \beta k)}.
\]

In fact, $f(t) = E_{\beta}(-\lambda t^{\beta})$ solves the eigenvalue equation

\[
\frac{\partial^{\beta} f(t)}{\partial t^{\beta}} = -\lambda f(t)
\]

for any $\lambda > 0$. This is easy to check, differentiating term-by-term and using the fact that $t^{p}$ has Caputo derivative $t^{p-\beta} \Gamma(p+1) / \Gamma(p+1-\beta)$ for $p > 0$ and $0 < \beta \leq 1$.

For $0 < \alpha < 2$, the fractional Laplacian $\Delta^{\alpha/2} f$ is defined for $f \in \text{Dom}(\Delta^{\alpha/2}) = \{ f \in L^2(\mathbb{R}^d; dx) : \int_{\mathbb{R}^d} |\xi|^\alpha |\hat{f}(\xi)|^2 d\xi < \infty \}$ as the function with Fourier transform

\[
\hat{\Delta^{\alpha/2} f}(\xi) = -|\xi|^\alpha \hat{f}(\xi).
\]

For suitable test functions (for example, $C^2$ functions with bounded second derivatives), the fractional Laplacian can be defined pointwise:

\[
\Delta^{\alpha/2} f(x) = \int_{y \in \mathbb{R}^d} \left( f(x+y) - f(x) - \nabla f(x) \cdot y 1_{\{|y| \leq 1\}} \right) \frac{c_{d,\alpha}}{|y|^{d+\alpha}} dy,
\]

where $c_{d,\alpha} > 0$ is a specific constant that depends on $d$ and $\alpha$ so that

\[
c_{d,\alpha} \int_{y \in \mathbb{R}^d} \frac{1 - \cos y_1}{|y|^{d+\alpha}} dy = 1.
\]

Remark 3.1. (i) It can be verified using Fourier transforms that, for $f \in \text{Dom}(\Delta^{\alpha/2})$, if the right hand side of $3.3$ is well-defined for a.e. $x \in \mathbb{R}^d$, then the Fourier transform of the right-hand side of $3.3$ equals $-|\xi|^\alpha \hat{f}(\xi)$ (cf. \[18\] Theorem 7.3.16]). Conversely, it can also be verified that if $f \in L^2(\mathbb{R}^d; dx)$ is a function such that the right hand side of $3.3$ is well-defined for a.e. $x \in \mathbb{R}^d$ and is $L^2(\mathbb{R}^d; dx)$-integrable, then $f \in \text{Dom}(\Delta^{\alpha/2})$ and $3.3$ holds.
(ii) Using a Taylor series expansion in \( (3.3) \), it is easy to see that \( \Delta^{\alpha/2}f(x_0) \) exists and is finite at a point \( x_0 \in \mathbb{R}^d \) if \( f \) is bounded on \( \mathbb{R}^d \) and \( f \) is \( C^2 \) at the point \( x_0 \). Hence, if \( f \) is bounded and continuous on \( \mathbb{R}^d \) and \( f \) is \( C^2 \) in an open set \( D \), then \( \Delta^{\alpha/2}f \) exists pointwise and is continuous in \( D \). Moreover, if \( f \) is a \( C^1 \) function on \( [0, \infty) \) with \( |f'(t)| \leq ct^{\gamma-1} \) for some \( \gamma > 0 \), then by \( (3.1) \), the Caputo fractional derivative \( \partial^\alpha f(t)/\partial t^\alpha \) of \( f \) exists for every \( t > 0 \) and the derivative is continuous in \( t > 0 \). \( \square \)

For \( 0 < \alpha \leq 2 \), let \( X \) be the Lévy process on \( \mathbb{R}^d \) such that

\[
\mathbb{E} \left[ e^{i\xi \cdot (x_t - x_0)} \right] = e^{-t|\xi|^{\alpha}} \quad \text{for every} \quad \xi \in \mathbb{R}^d.
\]

This Lévy process \( X \) is called a standard (rotationally) symmetric \( \alpha \)-stable process on \( \mathbb{R}^d \). When \( \alpha = 2 \), it is Brownian motion running at double speed.

Denote the transition semigroup of \( X \) by \( \{P_t, t > 0\} \). Using the fact that \( X_t \Rightarrow X_0 \) as \( t \to 0+ \), it is not hard to show (e.g., see [1, Theorem 13.4.2]) that \( \{P_t, t \geq 0\} \) is a symmetric strongly continuous semigroup on the Banach space \( L^2(\mathbb{R}^d; dx) \). Let \( (\mathcal{F}, \mathcal{E}) \) be the Dirichlet form of \( X \) on \( L^2(\mathbb{R}^d; dx) \). That is,

\[
\mathcal{F} = \left\{ u \in L^2(\mathbb{R}^d; dx) : \sup_{t > 0} \frac{1}{t} (u - P_t u, u)_{L^2(\mathbb{R}^d; dx)} < \infty \right\},
\]

\[
\mathcal{E}(u, v) = \lim_{t \to 0} \frac{1}{t} (u - P_t u, v)_{L^2(\mathbb{R}^d; dx)} \quad \text{for} \quad u, v \in \mathcal{F}.
\]

It is known that, for example, via Fourier transforms [14],

\[
\mathcal{F} = W^{\alpha/2,2}(\mathbb{R}^d) := \left\{ u \in L^2(\mathbb{R}^d; dx) : \int_{\mathbb{R}^d \times \mathbb{R}^d} \frac{(u(x) - u(y))^2}{|x - y|^{d+\alpha}} dx dy < \infty \right\},
\]

\[
\mathcal{E}(u, v) = \frac{c_{d, \alpha}}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d} \frac{(u(x) - u(y))(v(x) - v(y))}{|x - y|^{d+\alpha}} dx dy.
\]

Let \( (\text{Dom}(\mathcal{L}), \mathcal{L}) \) be the \( L^2 \)-generator of the Dirichlet form \( (\mathcal{E}, \mathcal{F}) \); that is, \( f \in \text{Dom}(\mathcal{L}) \) if and only if \( f \in W^{\alpha/2,2}(\mathbb{R}^d) \) and there is some \( u \in L^2(\mathbb{R}^d; dx) \) so that

\[
\mathcal{E}(f, g) = -(u, g) \quad \text{for every} \quad g \in W^{\alpha/2,2}(\mathbb{R}^d);
\]

in this case, we denote this \( u \) by \( \mathcal{L} f \). It is known (cf. [14]) that \( \mathcal{L} \) is also the semigroup generator of \( \{P_t, t > 0\} \) on the space \( L^2(\mathbb{R}^d; dx) \). Using the Fourier transform, one can conclude (cf. [14]) that \( f \in \text{Dom}(\mathcal{L}) \) if and only if \( \int_{\mathbb{R}^d} |\xi|^{\alpha} |\hat{f}(\xi)|^2 d\xi < \infty \), and \( \hat{\mathcal{L}} f(\xi) = -|\xi|^{\alpha} \hat{f}(\xi) \) for every \( f \in \text{Dom}(\mathcal{L}) \). Hence the \( L^2 \)-generator of \( X \) is the fractional Laplacian \( \Delta^{\alpha/2} \).

It follows directly from Dirichlet form theory (cf. [14]) that, for \( f \in L^2(\mathbb{R}^d) \) and \( t > 0 \), \( P_t f \in \mathcal{F} = W^{\alpha/2,2}(\mathbb{R}^d) \), and \( v(t, x) := \mathbb{E}_x[f(X_t)] \) is a weak solution to the following parabolic equation:

\[
\frac{\partial}{\partial t} v(t, x) = \Delta^{\alpha/2} v(t, x); \quad v(0, x) = f(x).
\]
That is, the function $x \mapsto v(x, t)$ belongs to the domain of the $L^2$ generator $\mathcal{L} = \Delta^{\alpha/2}$ for every $t > 0$, and equation (3.6) holds in the space $L^2(\mathbb{R}^d; dx)$. Here the fractional Laplacian and the first time derivative in (3.6) are defined in terms of the Banach space norm. For example, the time derivative is the limit of a difference quotient that converges in the $L^2$ sense, so it need not exist point-wise. The classical diffusion equation models the evolution of particles away from their starting point, due to molecular collisions. The space-fractional diffusion equation (3.6) models particle motions in a heterogeneous environment, where the probability of long particle jumps follows a power law [17].

For $0 < \alpha < 2$, the symmetric $\alpha$-stable process $X$ can be obtained from Brownian motion on $\mathbb{R}^d$ through subordination in the sense of Bochner [8]. Let $\{B_t, \mathbb{P}_x, x \in \mathbb{R}^d\}$ be Brownian motion on $\mathbb{R}^d$ with $\mathbb{P}_x(B_0 = x) = 1$ and $\mathbb{E}_0[B_tB_t'] = 2tI$, where $'$ denotes the transpose, and $I$ is the $d \times d$ identity matrix. For $0 < \alpha < 2$, let $Z_t$ be a standard stable subordinator with $Z_0 = 0$, whose Laplace transform is $E[e^{-sZ_t}] = e^{-ts^{\alpha/2}}$ for every $s, t > 0$. Then it is easy to verify, using Fourier transforms and a simple conditioning argument, that $B_{Z_t}$ is a symmetric $\alpha$-stable Lévy process starting from the origin that has the same distribution as $X$, with $X_0 = 0$. The process $X$ has a jointly continuous transition density function $p(t, x, y) = p_t(x - y)$ with respect to the Lebesgue measure in $\mathbb{R}^d$. That is,

$$\mathbb{P}_x(X_t \in A) = \int_A p(t, x, y)dy.$$  

Using the self-similarity of the stable process and its relation with Brownian motion through subordination, it is not hard to show that for $\alpha \in (0, 2)$ we have

$$p_t(x) = t^{-d/\alpha}p_1(t^{-1/\alpha}x) \leq t^{-d/\alpha}p_1(0) =: t^{-d/\alpha}M_{d,\alpha}, \quad t > 0, x \in \mathbb{R}^d.$$  

Another kind of time change relates to particle waiting times. Suppose $\{T_t, t \geq 0\}$ is a uniformly bounded strongly continuous semigroup on a Banach space $E$, with infinitesimal generator $(\mathcal{A}, \text{Dom}(\mathcal{A}))$. It is known that $v(t) = T_tf$ solves the Cauchy problem $\partial v/\partial t = \mathcal{A}v$ with $v(0) = f$ for any $f \in \text{Dom}(\mathcal{A})$ (see [2]). Let $Z$ be a standard $\beta$-stable subordinator independent of $X$, and recall that $E_0 = \inf\{s > 0 : Z_s > t\}$ is its inverse process. If $g_{\beta}(u)$ is the density of $Z_1$, then [3, Theorem 3.1] shows that another subordinated semigroup

$$R_tf = \int_0^\infty g_{\beta}(u)T_{(t/u)^{\beta}}f \, du$$  

yields solutions to the time-fractional Cauchy problem: $w(t) = R_tf$ solves

$$\frac{\partial^{\beta}}{\partial t^{\beta}}w(t) = \mathcal{A}w; \quad w(0) = f$$  

on the Banach space $E$ for any $f \in \text{Dom}(\mathcal{A})$. Applying this to the transition semigroup $\{P_t, t \geq 0\}$ of the symmetric $\alpha$-stable process $X$ on the space $L^2(\mathbb{R}^d; dx)$, one
sees that the process $Y_t = X_{E_t}$ can be used to solve the space-time diffusion equation on $\mathbb{R}^d$; that is, $w(t, x) = \mathbb{E}_x[f(Y_t)]$ is a weak solution for

$$
\frac{\partial^\beta}{\partial t^\beta} w(x, t) = \Delta^{\alpha/2} w(x, t); \quad w(x, 0) = f(x).
$$

That is, the function $x \mapsto w(x, t)$ belongs to the domain of the $L^2$ generator $\mathcal{L} = \Delta^{\alpha/2}$ for every $t > 0$, and equation (3.9) holds in the Banach space $L^2(\mathbb{R}^d; dx)$.

4. Eigenfunction Expansion for Bounded Domains

Let $D$ be a bounded open subset of $\mathbb{R}^d$. Recall that $X$ is a standard spherically symmetric stable process on $\mathbb{R}^d$, and define the first exit time

$$
\tau_D = \inf\{t \geq 0 : X_t \notin D\}.
$$

Let $X^D$ denote the process $X$ killed upon leaving $D$; that is, $X_t^D = X_t$ for $t < \tau_D$ and $X_t^D = \partial$ for $t \geq \tau_D$. Here $\partial$ is a cemetery point added to $D$. Throughout this paper, we use the convention that any real-valued function $f$ can be extended by taking $f(\partial) = 0$. The subprocess $X^D$ has a jointly continuous transition density function $p_D(t, x, y)$ with respect to the Lebesgue measure on $D$. In fact, by the strong Markov property of $X$, one has for $t > 0$ and $x, y \in D$,

$$
p_D(t, x, y) = p(t, x, y) - \mathbb{E}_x[p(t - \tau_D, X_{\tau_D}, y); \tau_D < t] \leq p(t, x, y).
$$

Denote by $\{P^D_t, t \geq 0\}$ the transition semigroup of $X^D$, that is

$$
P^D_t f(x) = \mathbb{E}_x[f(X^D_t)] = \int_D p_D(t, x, y)f(y)dy.
$$

The proof of the following facts can be found in [14]: The operators $\{P^D_t, t \geq 0\}$ form a symmetric strongly continuous contraction semigroup in $L^2(D; dx)$. Let $(\mathcal{E}^D, \mathcal{F}^D)$ denote the Dirichlet form of $X^D$, defined by (3.4)–(3.5) but with $\{P_t^D, t > 0\}$ in place of $\{P_t, t > 0\}$. Then $\mathcal{F}^D$ is the $\mathcal{E}^D_1$-completion of the space $C^\infty_c(D)$ of smooth functions with compact support in $D$, denoted by $W^{1,2}_0(D)$ in literature. Here $\mathcal{E}(u, u) = \mathcal{E}(u, u) + \int_{\mathbb{R}^d} u(x)^2 dx$. Moreover, $\mathcal{E}^D(u, v) = \mathcal{E}(u, v)$ for $u, v \in W^{1,2}_0(D)$.

Let $\mathcal{L}_D$ be the $L^2$-infinitesimal generator of $(\mathcal{E}^D, \mathcal{F}^D)$; that is, its domain $\text{Dom}(\mathcal{L}_D)$ consists all $f \in W^{1,2}_0(D)$ such that

$$
\mathcal{E}^D(f, g) = -(u, g)_{L^2(D; dx)} \quad \text{for every } g \in W^{1,2}_0(D);
$$

for some $u \in L^2(D; dx)$; in this case, we denote this $u$ by $\mathcal{L}_D f$. It is well-known (cf. [14]) that $\mathcal{L}_D$ is the $L^2$-generator of the strongly continuous semigroup $\{P^D_t, t > 0\}$ in $L^2(D; dx)$. For every $f \in L^2(D; dx)$ and $t > 0$, $P^D_t f \in \text{Dom}(\mathcal{L}_D) \subset W^{1,2}_0(D)$. Moreover $u(t, x) := P^D_t f(x)$ is the unique weak solution to

$$
\frac{\partial u}{\partial t} = \mathcal{L}_D u
$$

with initial condition $u(0, x) = f(x)$ on the Banach space $L^2(D; dx)$.
Note that the transition kernel $p_D(t, x, y)$ is symmetric and strictly positive with
\begin{equation}
4.2 \quad p_D(t, x, y) \leq p(t, x, y) \leq t^{-d/\alpha} M_{d, \alpha}, \quad x, y \in D, \quad t > 0
\end{equation}
in view of (3.7). In particular, one has $\sup_{x \in D} \int_D p(t, x, y) \, dy < \infty$ for every $t > 0$. Thus for each $t > 0$, $P^D_t$ is a Hilbert-Schmidt operator in $L^2(D; dx)$ so it is compact. Therefore there is a sequence of positive numbers $0 < \lambda_1 < \lambda_2 \leq \lambda_3 \leq \cdots$ and an orthonormal basis $\{\psi_n, n \geq 1\}$ of $L^2(D; dx)$ so that $P^D_t \psi_n = e^{-\lambda_n t} \psi_n$ in $L^2(D; dx)$ for every $n \geq 1$ and $t > 0$. Since for every $f \in L^2(D; dx)$, $f(x) = \sum_{n=1}^{\infty} \langle f, \psi_n \rangle \psi_n(x)$, we have
\begin{equation}
4.3 \quad P^D_t f(x) = \sum_{n=1}^{\infty} \langle f, \psi_n \rangle P^D_t \psi_n(x) = \sum_{n=1}^{\infty} e^{-\lambda_n t} \langle f, \psi_n \rangle \psi_n(x).
\end{equation}
That is, the transition density
\begin{equation}
4.4 \quad p_D(t, x, y) = \sum_{n=1}^{\infty} e^{-\lambda_n t} \psi_n(x) \psi_n(y).
\end{equation}
It follows from [7, Theorem 2.3] that for any bounded open subset $D$ of $\mathbb{R}^d$, one has
\begin{equation}
4.5 \quad c_1 n^{\alpha/d} \leq \lambda_n \leq c_2 n^{\alpha/d} \quad \text{for every } n \geq 1.
\end{equation}
Using the spectral representation, one has
\begin{equation}
4.6 \quad \text{Dom}(L_D) = \left\{ f \in L^2(D) : \|L_D f\|_{L^2(D)}^2 = \sum_{n=1}^{\infty} \lambda_n^2 \langle f, \psi_n \rangle^2 < \infty \right\}.
\end{equation}
and
\[ L_D f(x) = -\sum_{n=1}^{\infty} \lambda_n \langle f, \psi_n \rangle \psi_n(x) \quad \text{for } f \in \text{Dom}(L_D). \]
For any real valued function $\phi : \mathbb{R} \to \mathbb{R}$, one can also define the operator $\phi(L_D)$ as follows:
\[ \text{Dom}(\phi(L_D)) = \left\{ f \in L^2(D; dx) : \sum_{n=1}^{\infty} \phi(\lambda_n)^2 \langle f, \psi_n \rangle^2 < \infty \right\}, \]
\[ \phi(L_D) f = \sum_{n=1}^{\infty} \phi(\lambda_n) \langle f, \psi_n \rangle \psi_n. \]
In next section, the operator $L^k_D$ defined using $\phi(t) = t^k$ will be utilized.

The generator $L_D$ is also called the fractional Laplacian on $D$ with zero exterior condition, denoted as $\Delta^{\alpha/2}|_D$. We now record a lemma that gives an explicit expression of $L_D$. 

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Lemma 4.1. For $f \in \mathcal{F}^D$, if

$$
\phi(x) := \lim_{\varepsilon \to 0} \int_{\{y \in \mathbb{R}^d : |y-x| > \varepsilon\}} (f(y) - f(x)) \frac{c_{d,\alpha}}{|y-x|^{d+\alpha}} dy
$$

exists and the convergence is uniformly on each compact subsets of $D$ and $\phi \in L^2(D; dx)$, then $f \in \text{Dom}(\mathcal{L}_D)$ and $\phi = \mathcal{L}_D f$. In particular, if $f$ is a bounded function in $\mathcal{F}^D \cap C^2(D)$, then $f \in \text{Dom}(\mathcal{L}_D)$ and

$$
\mathcal{L}_D f(x) = \lim_{\varepsilon \to 0} \int_{\{y \in \mathbb{R}^d : |y-x| > \varepsilon\}} (f(y) - f(x)) \frac{c_{d,\alpha}}{|y-x|^{d+\alpha}} dy
$$

$$
= \int_{\mathbb{R}^d} (f(x+y) - f(x) - \nabla f(x) \cdot y \mathbf{1}_{\{|y| \leq 1\}}) \frac{c_{d,\alpha}}{|y|^{d+\alpha}} dy.
$$

Proof. Suppose that $f \in \mathcal{F}^D$ and that $\phi$ defined by (4.7) converges locally uniformly in $D$ and is in $L^2(D; dx)$. Then for every $g \in C^2_c(D)$, by the expression of $\mathcal{E}_D(f, g)$ and the symmetry,

$$
\mathcal{E}_D(f, g) = \frac{1}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d} (f(x) - f(y))(g(x) - g(y)) \frac{c_{d,\alpha}}{|x-y|^{d+\alpha}} dx dy
$$

$$
= \frac{1}{2} \int_{\mathbb{R}^d} \left( \int_{\mathbb{R}^d} (f(y) - f(x))(g(y) - g(x)) \frac{c_{d,\alpha}}{|y-x|^{d+\alpha}} dy \right) g(x) dx
$$

$$
= -\int_{\mathbb{R}^d} \phi(x) g(x) dx.
$$

Since $C^2_c(D)$ is $\mathcal{E}_1^D$-dense in $W^{\alpha/2,2}_0(D)$, this implies that $f \in \text{Dom}(\mathcal{L}_D)$ and $\mathcal{L}_D f = \phi$ on $D$.

Assume now that $f$ is a bounded function in $\mathcal{F}^D \cap C^2(D)$. Using a Taylor expansion, one easily sees that

$$
\int_{y \in \mathbb{R}^d} |f(x+y) - f(x) - \nabla f(x) \cdot y \mathbf{1}_{\{|y| \leq 1\}}| \frac{c_{d,\alpha}}{|y|^{d+\alpha}} dy < \infty \quad \text{for every } x \in D
$$

and the integral is a continuous function on $D$. Set

$$
\psi(x) = \int_{y \in \mathbb{R}^d} (f(x+y) - f(x) - \nabla f(x) \cdot y \mathbf{1}_{\{|y| \leq 1\}}) \frac{c_{d,\alpha}}{|y|^{d+\alpha}} dy \quad \text{for } x \in D.
$$

For any compact subset $K$ of $D$, let

$$
K_\varepsilon := \{ z \in \mathbb{R}^d : \text{there is some } x \in K \text{ so that } |z-x| \leq \varepsilon \}.
$$

Defining

$$
\|D^2 f\|_\infty = \max_{1 \leq i,j \leq d} \left\| \frac{\partial^2 f}{\partial x_i \partial x_j} \right\|_\infty,
$$


we have
\[
\lim_{\varepsilon \to 0} \sup_{x \in K} \left| \int_{\{y \in \mathbb{R}^d : |y - x| > \varepsilon \}} (f(y) - f(x)) \frac{c_{d,\alpha}}{|y - x|^{d+\alpha}} dy - \psi(x) \right|
\]
\[
= \lim_{\varepsilon \to 0} \sup_{x \in K} \left| \int_{\{y \in \mathbb{R}^d : |y - x| \leq \varepsilon \}} (f(x + y) - f(x) - \nabla f(x) \cdot y 1_{\{|y| \leq 1\}}) \frac{c_{d,\alpha}}{|y|^{d+\alpha}} dy \right|
\]
\[
\leq \lim_{\varepsilon \to 0} \left| \int_{\{y \in \mathbb{R}^d : |y - x| \leq \varepsilon \}} \sup_{z \in K_{\varepsilon}} \|D^2 f\|_{\infty} |y|^{2} \frac{c_{d,\alpha}}{|y|^{d+\alpha}} dy \right| = 0.
\]
By what we have shown in the first part, this implies that \( f \in \text{Dom}(\mathcal{L}_D) \) with \( \mathcal{L}_D f = \psi \), which completes the proof of the lemma.

The main purpose of this paper is to investigate the existence of strong solution to the following equation:
\[
\frac{\partial^{\beta}}{\partial t^{\beta}} u(t, x) = \Delta^{\alpha/2} u(t, x); \quad x \in D, \ t > 0
\]
(4.8)
\[
u(t, x) = 0, \quad x \in D^c, \ t > 0,
\]
\[
u(0, x) = f(x), \quad x \in D.
\]
Let \( C_\infty(D) \) denote the Banach space of bounded continuous functions on \( \mathbb{R}^d \) that vanish off \( D \), with the sup norm.

**Definition 4.2.** (i) Suppose that \( f \in L^2(D; dx) \). A function \( u(t, x) \) is said to be a weak solution to (4.8) if \( u(t, \cdot) \in W_{0}^{1,2}(D) \) for every \( t > 0 \), \( \lim_{t \downarrow 0} u(t, x) = f(x) \) a.e. in \( D \), and \( \partial^{\beta}/\partial t^{\beta} u(t, x) = \Delta^{\alpha/2} u(t, x) \) in the distributional sense; that is, for every \( \psi \in C_c([0, \infty)) \) and \( \phi \in C_c^2(D) \),
\[
\int_{\mathbb{R}^d} \left( \int_{0}^{\infty} u(t, x) \frac{\partial^{\beta}}{\partial t^{\beta}} \psi(t) dt \right) \phi(x) dx = \int_{0}^{\infty} \mathcal{E}^{D}(u(t, \cdot), \phi) \psi(t) dt.
\]
(ii) Suppose that \( f \in C(D) \). A function \( u(t, x) \) is said to be a strong solution (4.8) if for every \( t > 0 \), \( u(t, \cdot) \in C_\infty(D) \), \( \Delta^{\alpha/2} u(t, \cdot)(x) \) exists pointwise for every \( x \in D \) in the sense of (3.3), the Caputo fractional derivative \( \partial^{\beta} u(t, x)/\partial t^{\beta} \) exists pointwise for every \( t > 0 \) and \( x \in D \), \( \partial^{\beta}/\partial t^{\beta} u(t, x) = \Delta^{\alpha/2} u(t, x) \) pointwise in \((0, \infty) \times D \), and \( \lim_{t \downarrow 0} u(t, x) = f(x) \) for every \( x \in D \).

A boundary point \( x \) of an open set \( D \) is said to be regular for \( D \) if \( \mathbb{P}_x[\tau_D(X) = 0] = 0 \).

A sufficient condition for \( x_0 \in \partial D \) to be regular for \( D \) is that \( D \) satisfies an *exterior cone condition* at \( x_0 \), that is, there exists a finite right circular open cone \( V = V_{x_0} \) with vertex \( x_0 \) such that \( V_{x_0} \subset D^c \) (cf. [10] Theorem 2.2]. An open set \( D \) is said to be regular if every boundary point of \( D \) is regular for \( D \). Assume now that \( D \) is a regular open set. Then [10] Theorem 2.3] shows that \( \{P_t^D, t > 0\} \) is a strongly continuous (Feller) semigroup on the Banach space \( C_\infty(D) \) of bounded continuous functions on \( \mathbb{R}^d \) that vanish off \( D \), with the sup norm. Moreover, \( \{P_t^D, t > 0\} \) has the same
set of eigenvalues and eigenfunctions on $C_\infty(D)$ as on $L^2(D; dx)$: $P^D_t \psi_n = e^{-\lambda_n t} \psi_n$ in $C_\infty(D)$ (see [10, Theorem 3.3]). In particular, every eigenfunction $\psi_n$ of the $L^2$-generator $L_D$ is a bounded continuous function on $D$ that vanishes continuously on the boundary $\partial D$.

5. Space-time fractional diffusion in bounded domains

In this section, we prove strong solutions to space-time fractional diffusion equations on bounded domains in $\mathbb{R}^d$. We give an explicit solution formula, based on the solution of the corresponding Cauchy problem. The basic argument uses an eigenfunction expansion of the fractional Laplacian on $D$, and separation of variables. The probabilistic representation of the solution is constructed from a killed stable processes, whose index corresponds to the fractional Laplacian, modified by an inverse stable time change, whose index equals the order of the fractional time derivative.

Recall that $X$ is a rotationally symmetric $\alpha$-stable process in $\mathbb{R}^d$ and $\{E_t, t \geq 0\}$ is the inverse of a standard stable subordinator of index $\beta \in (0, 1)$, independent of $X$. In the following proof, we denote by $c, c_1, c_2, \ldots$ a constant that may change from line to line.

**Theorem 5.1.** Let $D$ be a regular open subset of $\mathbb{R}^d$. Suppose $f \in \text{Dom}(L^k_D)$ for some $k > -1 + (3d + 4)/(2\alpha)$. Then

$$u(t,x) = \mathbb{E}_x[f(X_{E_t}^D)] \in C_\infty([0, \infty) \times \mathbb{R}^d) \cap C^{1,2}((0, \infty) \times D)$$

and $u(t,x)$ is a strong solution to the space-time fractional diffusion equation (4.8).

**Proof.** First we will prove that $f \in C_\infty(D)$. Let $0 < \lambda_1 < \lambda_2 \leq \lambda_3 \leq \cdots$ be the eigenvalues of $L_D$ and $\{\psi_n, n \geq 1\}$ be the corresponding eigenfunctions, which form an orthonormal basis for $L^2(D; dx)$. Note that, since $D$ is a regular open set, we have from the last section that $\psi_n \in C_\infty(D)$ for each $n \geq 1$. Since $f \in \text{Dom}(L^k_D)$ for some $k > -1 + (3d + 4)/(2\alpha)$, using (4.5) it follows that

$$M := \sum_{n=1}^{\infty} \lambda_n^{2k} (f, \psi_n)^2 < \infty,$$

and so $|\langle f, \psi_n \rangle| \leq \sqrt{M} \lambda_n^{-k}$. From (4.2) and (4.4) we get

$$e^{-\lambda_n t} |\psi_n(x)|^2 \leq \sum_{k=1}^{\infty} e^{-\lambda_k t} |\psi_k(x)|^2 = p_D(t, x, x) \leq M_{d,\alpha} t^{-d/\alpha}$$

and hence, taking square roots of both sides, we get

$$|\psi_n(x)| \leq e^{\lambda_n t/2} \sqrt{M_{d,\alpha} t^{-d/\alpha}}$$

Taking $t = 1/\lambda_n$ gives us

$$|\psi_n(x)| \leq c \lambda_n^{d/(2\alpha)}$$

for every $x \in D$.
for some $c > 0$. Since $k > -1 + (3d + 4)/(2\alpha)$, (5.2) together with (4.5) implies that
\[
\sum_{n=1}^{\infty} |\langle f, \psi_n \rangle| \|\psi_n\|_\infty \leq c \sum_{n=1}^{\infty} \lambda_n^{-k} \lambda_n^{d/(2\alpha)} \leq c \sum_{n=1}^{\infty} n^{(\alpha/d)(d/(2\alpha)-k)} < \infty.
\]
Hence $f(x) = \sum_{n=1}^{\infty} \langle f, \psi_n \rangle \psi_n$ converges uniformly on $D$, and so $f \in C_\infty(D)$.

Recall that $P_t^D f(x) = \mathbb{E}_x[f(X_t^D)]$ is the unique weak solution in $W_0^{\alpha/2,2}(D)$ of the equation
\[
\frac{\partial}{\partial t} v(t, x) = \Delta^{\alpha/2} v(t, x) \quad \text{with } v(0, x) = f(x)
\]
on the Banach space $L^2(\mathbb{R}^d, dx)$ (cf. (see [14]). The semigroup $P_t^D$ has density function $p_D(t, x, y)$ given by (4.1). Note that $p(t, x, y)$ is smooth in $x$. By a proof similar to [5, Proposition 3.3], we have for every $j \geq 1$ and $1 \leq i \leq d$ that
\[
\left| \frac{\partial^j}{\partial x_i^j} p(t, x, y) \right| \leq c \left( t^{-(d+j)/\alpha} \land \frac{t}{|x-y|^{d+\alpha+j}} \right) \leq c_1 t^{-j/\alpha} p(t, x, y).
\]
In view of the symmetry $p(t, x, y) = p(t, y, x)$ and $p_D(t, x, y) = p_D(t, y, x)$, we have from (4.1) and (5.4) that $P_t^D f(x) = \int_D p_D(t, x, y) f(y) dy$ is smooth in $x \in D$. Moreover, for every compact subset $K$ of $D$ and $T > 0$, there is a constant $c_2 = c_2(d, \alpha, K, T)$ such that, for $x \in K$ and $t \in (0, T]$,
\[
\left| \frac{\partial^j}{\partial x_i^j} p_D(t, x, y) \right| \leq c_2 t^{-j/\alpha} p(t, x, y).
\]
The Chapman-Kolmogorov equation implies
\[
\int_{\mathbb{R}^d} p(t, x, y)^2 dy = \int_{\mathbb{R}^d} p(t, x, y)p(t, y, x) dy = p(2t, x, x).
\]
It then follows using (4.2), (5.5), and the Cauchy-Schwarz inequality that
\[
|\nabla^j P_t^D f(x)| \leq c_3 t^{-j/\alpha} (2t)^{-d/(2\alpha)} \|f\|_{L^2(D)}.
\]
Consequently, each eigenfunction $\psi_n(x) = e^{\lambda_n t} P_t^D \psi_n(x)$ is smooth inside $D$ with
\[
|\nabla^j \psi_n(x)| \leq c_3 t^{-(d+2j)/(2\alpha)} e^{\lambda_n t}
\]
for $x \in K$ and $t \in (0, T]$. Taking $t = 1/\lambda_n$ yields
\[
|\nabla^j \psi_n(x)| \leq c_3 \lambda_n^{(d+2j)/(2\alpha)} \quad \text{for } x \in K.
\]
In view of (4.3), $P_t^D f(x)$ is also differentiable in $t > 0$. (The eigenfunction expansion (4.3) together with (5.7) gives another proof that $P_t^D f$ is $C_\infty$ in $x \in D$.) Hence in view of Remark 3.1, $v(t, x) = P_t^D f(x)$ is a classical solution for $\partial v/\partial t = \mathcal{L}_D v$ in $D$.

Now define
\[
u(t, x) = \mathbb{E}_x[f(X_{E_t}^D)] = \mathbb{E}_x[f(\psi_n(x)) | E_t | \tau_D].
\]
Since $X^D$ generates a strongly continuous (Feller) semigroup on $C_{\infty}(D)$, $P_t^D f(x)$ is a bounded continuous function on $[0, \infty) \times \mathbb{R}^d$ that vanishes on $[0, \infty) \times D^c$, and hence so is $u$, in view of (3.8). By [3, Theorem 3.1] (and [20, Theorem 4.2]), $u(t,x)$ is a weak solution for the parabolic equation (3.8) on $L^2(\mathbb{R}^d, dx)$. Then, to show that $u$ is a classical solution, by Remark 3.1, it suffices to show that $u(t,\cdot) \in C^2(D)$ for each $t > 0$, and that the Caputo derivative of $t \mapsto u(t,x)$ exists for each $x$, and is jointly continuous in $(t,x)$.

Bingham [6] showed that the inverse stable law $E_t$ with density $f_t(s)$ given by (2.1) has a Mittag-Leffler distribution, with Laplace transform $E[\text{e}^{-\lambda E_t}] = E_\beta(-\lambda t^\beta)$. Then it follows, using (4.3) and a simple conditioning argument, that

$$u(t,x) = \int_0^\infty \mathbb{E}_x [f(X_s); s < \tau_D] f_t(s) \, ds = \int_0^\infty \left( \sum_{n=1}^\infty e^{-s\lambda_n} \langle f, \psi_n \rangle \psi_n(x) \right) f_t(s) \, du = \sum_{n=1}^\infty E_\beta(-\lambda_n t^\beta) \langle f, \psi_n \rangle \psi_n(x).$$

Then, since $0 \leq E_\beta(-\lambda_n t^\beta) \leq c/(1 + \lambda_n t^\beta)$, we have by (5.7) and (5.8) that

$$\|\nabla^j u\|_\infty \leq \sum_{n=1}^\infty E_\beta(-\lambda_n t^\beta) \langle f, \psi_n \rangle \|\nabla^j \psi_n\|_\infty \leq \sum_{n=1}^\infty c \lambda_n^{-k} \sqrt{M} \lambda_n^{(d+4)/(2\alpha)} 1 + \lambda_n t^\beta \leq (c \sqrt{M}) t^{-\beta} \sum_{n=1}^\infty \lambda_n^{(d+4)/(2\alpha) - 1 - k}$$

for $j = 1, 2$. Then by (4.5),

$$\|\nabla^j u\|_\infty \leq (c \sqrt{M}) t^{-\beta} \sum_{n=1}^\infty \lambda_n^{(d+4)/(2\alpha) - 1 - k} \leq (cc_n \sqrt{M}) t^{-\beta} \sum_{n=1}^\infty n^{(\alpha/d)((d+4)/(2\alpha) - 1 - k)} < \infty$$

if $k > (3d + 4 - 2\alpha)/(2\alpha)$. This proves that, when $k > -1 + (3d + 4)/(2\alpha)$, $u(t,x)$ is $C^2$ in $x \in K$, and hence in $D$. Consequently, by Remark 3.1, the spatial fractional derivative $\Delta^{\alpha/2} u(t,x)$ exists pointwise for $x \in D$, and is a jointly continuous function in $(t,x)$. 


Next we show $u(t, x)$ is $C^1$ in $t > 0$. Let $0 < \gamma < 1 \wedge (4/(2\alpha) - 1)$. By [16, Equation (17)],

\[
\left| \frac{\partial}{\partial t} E_\beta(-\lambda_n t^\beta) \right| \leq c \frac{\lambda_n^\gamma t^{\gamma\beta - 1}}{1 + \lambda_n t^\beta} \leq c \lambda_n^\gamma t^{\gamma\beta - 1}.
\]

This together with (5.1) and (5.2) yields that

\[
\sum_{n=1}^{\infty} \left| \frac{\partial}{\partial t} E_\beta(-\lambda_n t^\beta) \langle f, \psi_n \rangle \psi_n(x) \right| \leq \sum_{n=1}^{\infty} c \lambda_n^\gamma t^{\gamma\beta - 1} \lambda_n^{-k} \lambda_n^{d/(2\alpha)}
\]

\[
\leq ct^{\gamma\beta - 1} \sum_{n=1}^{\infty} n^{(\alpha/d)(\gamma-k+d/(2\alpha))} \leq c t^{\gamma\beta - 1}.
\]

Then it follows by a dominated convergence argument that $u(t, x)$ is continuously differentiable in $t > 0$, with

\[
(5.9) \quad \left| \frac{\partial u(t, x)}{\partial t} \right| \leq \sum_{n=1}^{\infty} \left| \frac{\partial}{\partial t} E_\beta(-\lambda_n t^\beta) \langle f, \psi_n \rangle \psi_n(x) \right| < ct^{\gamma\beta - 1} \quad \text{for every } x \in D.
\]

Hence by Remark 3.1, The Caputo fractional derivative $\partial^\beta u(t, x)/\partial t^\beta$ of $u(t, x)$ exists pointwise and is jointly continuous in $(t, x)$. Since $u(t, x)$ is a weak solution of (4.8) on $L^2(\mathbb{R}^d; dx)$, by the above regularity property of $u(t, x)$, it is also a strong solution of (4.8). □

Remark 5.2. The above proof can be easily modified to show that, if $D$ is a bounded regular open subset of $\mathbb{R}^d$ and $f \in \text{Dom}(\mathcal{L}_D^k)$ for some $k > 1+(3d)/(2\alpha)$, then $u(t, x) = \mathbb{E}_x[f(X_{E_t}^D)]$ is a weak solution to the space-time fractional diffusion equation (4.8). Moreover, the Caputo derivative $\partial^\beta u/\partial t^\beta$ exists pointwise as a jointly continuous function in $(t, x)$, and $\mathcal{L}_D u$ has a continuous version that equals $\partial^\beta u/\partial t^\beta$ on $(0, \infty) \times D$.

Remark 5.3. The paper [22] solves distributed-order time-fractional diffusion equations $\partial^\nu_t u = \Delta u$ on bounded domains. The distributed-order time-fractional derivative is defined by

\[
\partial^\nu_t f(t) = \int \frac{\partial^\nu f(t)}{\partial t^\beta} \nu(d\beta),
\]

where $\nu$ is a positive measure on $(0, 1)$. It may also be possible to extend the results of this paper to develop strong solutions and probabilistic solutions for $\partial^\nu_t u = \Delta^{\alpha/2} u$ on bounded domains. Distributed-order time-fractional diffusion equations can be used to model ultraslow diffusion, in which a cloud of particles spreads at a logarithmic rate, also called Sinai diffusion [21]. □
Remark 5.4. The fractional Laplacian generates the simplest non-Gaussian stable process in $\mathbb{R}^d$. Stable processes are useful in applications because they represent universal random walk limits. For random walks with strongly asymmetric jumps, a wide variety of alternative limit processes exists, see for example [18]. Because the generators of these processes are not self-adjoint, the extension of results in this paper to that case remains a challenging open problem.

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