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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 [1,2]. 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 [3]. 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 [4,5]. 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.

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

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represents the location of a random particle at time n. Suppose the distribution of Y is spherically symmetric. If $\sigma^2 := \mathbb{E}\left[|Y_1|^2\right]$ is finite and $\mathbb{E}[Y_1] = 0$, Donsker's invariance principle implies that as $\lambda \to \infty$, the random process $\{\lambda^{-1/2} S_{\lambda t}, t \geq 0\}$ converges weakly in the Skorohod space to a Brownian motion $\{B_t, t \geq 0\}$ with $\mathbb{E}[B_1^2] = \sigma^2$. 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 $\mathbb{E}\left[|Y_1|^2\right]$ is infinite, and the extended central limit theorem tells us that $\{\lambda^{-1/\alpha} S_{\lambda t}, t \geq 0\}$ converges weakly to a rotationally symmetric α-stable Lévy motion $\{A_t, t \geq 0\}$ with

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

where the constant C_0 depends only on α, C, and the dimension d, see [6]. A simple rescaling in space yields a standard stable process with $C_0 = 1$. Since $\{\lambda^{1/\alpha} A_t, t \geq 0\}$ has the same distribution as $\{A_{\lambda t}, t \geq 0\}$, stable Lévy motion represents a model for anomalous super-diffusion, where particles spread faster than a Brownian motion [7].

If we impose a random waiting time T_n before the nth 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 time-changed process. If $\mathbb{P}(J_n > t) \sim Ct^{-\beta}$ as $t \to \infty$ for some $0 < \beta < 1$, then the scaling limit of $c^{-1/\beta} T_{[ct]} \Rightarrow Z_t$ as $c \to \infty$ is a strictly increasing stable Lévy motion with index β, sometimes called a stable subordinator. The jump times T_n and the number of jumps N_t are inverses: $\{N_t \geq n\} = \{T_n \leq t\}$. [8, Theorem 3.2] shows that $\{c^{-\beta} N_{ct}, t \geq 0\}$ 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 [8, 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

$$f_t(s) = \frac{d}{ds} \mathbb{P}(Z_s \geq t) = t\beta^{-1} s^{-1-1/\beta} g_\beta(ts^{-1/\beta}). \tag{2.1}$$

For more details, see [3,8].

3. Fractional calculus

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

$$\frac{\partial^\beta f(t)}{\partial t^\beta} = \frac{1}{\Gamma(1-\beta)} \int_0^t \frac{\partial f(r)}{\partial r} \frac{dr}{(t-r)^\beta}, \tag{3.1}$$

was invented to properly handle initial values [9,10]. 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 [4,11]. 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

$$f \in \mathrm{Dom}(\Delta^{\alpha/2}) = \left\{ f \in L^2(\mathbb{R}^d; dx) : \int_{\mathbb{R}^d} |\xi|^\alpha \, |\widehat{f}(\xi)|^2 d\xi < \infty \right\}$$

as the function with Fourier transform

$$\widehat{\Delta^{\alpha/2} f}(\xi) = -|\xi|^\alpha \widehat{f}(\xi). \tag{3.2}$$

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

$$\Delta^{\alpha/2} f(x) = \int_{y \in \mathbb{R}^d} \left(f(x+y) - f(x) - \nabla f(x) \cdot y \mathbf{1}_{\{|y| \leq 1\}} \right) \frac{c_{d,\alpha}}{|y|^{d+\alpha}} \, dy, \tag{3.3}$$

where $c_{d,\alpha} > 0$ is a specific constant that depends on d and α 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 $f \in \mathrm{Dom}(\Delta^{\alpha/2})$, 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 $-|\xi|^\alpha \widehat{f}(\xi)$ (cf. [6, 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 $f \in \mathrm{Dom}(\Delta^{\alpha/2})$ 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 $|f'(t)| \le c\, t^{\gamma-1}$ for some $\gamma > 0$, then by (3.1), the Caputo fractional derivative $\partial^\beta f(t)/\partial t^\beta$ of f exists for every $t > 0$ and the derivative is continuous in $t > 0$. □

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

$$\mathbb{E}\left[e^{i\xi\cdot(X_t - X_0)}\right] = e^{-t|\xi|^\alpha} \quad \text{for every } \xi \in \mathbb{R}^d.$$

This Lévy process X is called a standard (rotationally) symmetric α-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 [12, Theorem 13.4.2]) that $\{P_t, t \ge 0\}$ is a symmetric strongly continuous semigroup on the Hilbert 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,

$$\mathcal{F} = \left\{ u \in L^2(\mathbb{R}^d; dx) : \sup_{t>0} \frac{1}{t}(u - P_t u, u)_{L^2(\mathbb{R}^d; dx)} < \infty \right\}, \tag{3.4}$$

$$\mathcal{E}(u, v) = \lim_{t \to 0} \frac{1}{t}(u - P_t u, v)_{L^2(\mathbb{R}^d; dx)} \quad \text{for } u, v \in \mathcal{F} \tag{3.5}$$

It is known that, for example, via Fourier transforms [13],

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

$$\mathcal{E}(u, v) = \frac{c_{d,\alpha}}{2} \int_{\mathbb{R}^d \times \mathbb{R}^d} \frac{(u(x) - u(y))(v(x) - v(y))}{|x - y|^{d+\alpha}} dxdy \quad \text{for } u, v \in \mathcal{F}.$$

Let $(\mathrm{Dom}(\mathcal{L}), \mathcal{L})$ be the L^2-generator of the Dirichlet form $(\mathcal{E}, \mathcal{F})$; that is, $f \in \mathrm{Dom}(\mathcal{L})$ 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

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

in this case, we denote this u by $\mathcal{L}f$. It is known (cf. [13]) 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. [13]) that $f \in \mathrm{Dom}(\mathcal{L})$ if and only if $\int_{\mathbb{R}^d} |\xi|^\alpha |\widehat{f}(\xi)|^2 d\xi < \infty$, and $\widehat{\mathcal{L}f}(\xi) = -|\xi|^\alpha \widehat{f}(\xi)$ for every $f \in \mathrm{Dom}(\mathcal{L})$. Hence the L^2-generator of X is the fractional Laplacian $\Delta^{\alpha/2}$.

It follows directly from Dirichlet form theory (cf. [13]) 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:

$$\frac{\partial}{\partial t} v(t, x) = \Delta^{\alpha/2} v(t, x); \qquad v(0, x) = f(x). \tag{3.6}$$

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 Eq. (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 Hilbert 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 [7].

For $0 < \alpha < 2$, the symmetric α-stable process X can be obtained from Brownian motion on $\mathbb{R}^d$ through subordination in the sense of Bochner [14]. Let $\{B, \mathbb{P}_x, x \in \mathbb{R}^d\}$ be Brownian motion on $\mathbb{R}^d$ with $\mathbb{P}_x(B_0 = x) = 1$ and $\mathbb{E}_0[B_t B_t'] = 2tI$, 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 $\mathbb{E}[e^{-sZ_t}] = e^{-ts^{\alpha/2}}$ 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 α-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

$$p_t(x) = t^{-d/\alpha} p_1(t^{-1/\alpha} x) \le t^{-d/\alpha} p_1(0) =: t^{-d/\alpha} M_{d,\alpha}, \quad t > 0, x \in \mathbb{R}^d. \tag{3.7}$$

Another kind of time change relates to particle waiting times. Suppose $\{T_t, t \ge 0\}$ is a uniformly bounded strongly continuous semigroup on a Banach space E, with infinitesimal generator $(\mathcal{A}, \mathrm{Dom}(\mathcal{A}))$. It is known that $v(t) = T_t f$ solves the Cauchy problem $\partial v/\partial t = \mathcal{A} v$ with $v(0) = f$ for any $f \in \mathrm{Dom}(\mathcal{A})$ (see [15]). Let Z be a standard β-stable subordinator independent of X, and recall that $E_t = \inf\{s > 0 : Z_s > t\}$ is its inverse process. If $g_\beta(u)$ is the density of Z_1, then [16, Theorem 3.1] shows that the time-changed semigroup

$$R_t f = \int_0^\infty g_\beta(u) T_{(t/u)^\beta} f \, du \tag{3.8}$$

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

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

on the Banach space E for any $f \in \mathrm{Dom}(\mathcal{A})$. Applying this to the transition semigroup $\{P_t, t \ge 0\}$ of the symmetric α-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

$$\frac{\partial^\beta}{\partial t^\beta} w(x, t) = \Delta^{\alpha/2} w(x, t); \qquad w(x, 0) = f(x). \tag{3.9}$$

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 Eq. (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 α-stable process on $\mathbb{R}^d$, and define the first exit time

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

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 $t \ge \tau_D$. Here ∂ 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 $x, y \in D$,

$$p_D(t, x, y) = p(t, x, y) - \mathbb{E}_x[p(t - \tau_D, X_{\tau_D}, y); \tau_D < t] \le p(t, x, y). \tag{4.1}$$

Denote by $\{P_t^D, t \ge 0\}$ the transition semigroup of X^D, that is

$$P_t^D f(x) = \mathbb{E}_x[f(X_t^D)] = \int_D p_D(t, x, y) f(y) dy.$$

The proof of the following facts can be found in [13]: The operators $\{P_t^D, t \ge 0\}$ 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 $\sqrt{\mathcal{E}_1}$-completion of the space $C_c^\infty(D)$ of smooth functions with compact support in D, denoted by $W_0^{\alpha/2,2}(D)$ in literature. Here $\mathcal{E}_1(u, u) = \mathcal{E}(u, u) + \int_{\mathbb{R}^d} u(x)^2 dx$. Moreover, $\mathcal{E}^D(u, v) = \mathcal{E}(u, v)$ for $u, v \in W_0^{\alpha/2,2}(D)$. Let $\mathcal{L}_D$ be the L^2-infinitesimal generator of $(\mathcal{E}^D, \mathcal{F}^D)$; that is, its domain $\mathrm{Dom}(\mathcal{L}_D)$ consists all $f \in W_0^{\alpha/2,2}(D)$ such that

$$\mathcal{E}^D(f, g) = -(u, g)_{L^2(D;dx)} \quad \text{for every } g \in W_0^{\alpha/2,2}(D);$$

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. [13]) that $\mathcal{L}_D$ is the L^2-generator of the strongly continuous semigroup $\{P_t^D, t > 0\}$ in $L^2(D; dx)$. For every $f \in L^2(D; dx)$ and $t > 0$, $P_t^D f \in \mathrm{Dom}(\mathcal{L}_D) \subset W_0^{\alpha/2,2}(D)$. Moreover $u(t, x) := P_t^D f(x)$ 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 Hilbert space $L^2(D; dx)$.

Note that the transition kernel $p_D(t, x, y)$ is symmetric and strictly positive with

$$p_D(t, x, y) \le p(t, x, y) \le t^{-d/\alpha} M_{d,\alpha}, \quad x, y \in D, t > 0 \tag{4.2}$$

in view of (3.7). In particular, one has $\sup_{x\in D} \int_D p(t, x, y)^2 dy < \infty$ for every $t > 0$. Thus for each $t > 0$, P_t^D is a Hilbert–Schmidt operator in $L^2(D; dx)$ so it is compact. Therefore there is a sequence of positive numbers $0 < \lambda_1 < \lambda_2 \le \lambda_3 \le \cdots$ and an orthonormal basis $\{\psi_n, n \ge 1\}$ of $L^2(D; dx)$ so that $P_t^D \psi_n = e^{-\lambda_n t}\psi_n$ in $L^2(D; dx)$ for every $n \ge 1$ 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

$$P_t^D f(x) = \sum_{n=1}^{\infty} \langle f, \psi_n\rangle P_t^D \psi_n(x) = \sum_{n=1}^{\infty} e^{-\lambda_n t} \langle f, \psi_n\rangle \psi_n(x). \tag{4.3}$$

Consequently, the transition density

$$p_D(t, x, y) = \sum_{n=1}^{\infty} e^{-\lambda_n t} \psi_n(x)\psi_n(y). \tag{4.4}$$

It follows from [17, Theorem 2.3] that for any bounded open subset D of $\mathbb{R}^d$, one has

$$c_1 n^{\alpha/d} \le \lambda_n \le c_2 n^{\alpha/d} \quad \text{for every } n \ge 1. \tag{4.5}$$

Using the spectral representation, one has

$$\mathrm{Dom}(\mathcal{L}_D) = \left\{ f \in L^2(D) : \|\mathcal{L}_D f\|_{L^2(D)}^2 = \sum_{n=1}^{\infty} \lambda_n^2 \langle f, \psi_n\rangle^2 < \infty \right\} \tag{4.6}$$

and

$$\mathcal{L}_D f(x) = -\sum_{n=1}^{\infty} \lambda_n \langle f, \psi_n\rangle \psi_n(x) \quad \text{for } f \in \mathrm{Dom}(\mathcal{L}_D).$$

For any real valued function $\phi : \mathbb{R} \to \mathbb{R}$, one can also define the operator $\phi(\mathcal{L}_D)$ as follows:

$$\mathrm{Dom}(\phi(\mathcal{L}_D)) = \left\{ f \in L^2(D; dx) : \sum_{n=1}^{\infty} \phi(\lambda_n)^2 \langle f, \psi_n\rangle^2 < \infty \right\},$$

$$\phi(\mathcal{L}_D) f = \sum_{n=1}^{\infty} \phi(\lambda_n) \langle f, \psi_n\rangle \psi_n.$$

In next section, the operator $\mathcal{L}_D^k$ defined using $\phi(t) = t^k$ will be utilized.

The generator $\mathcal{L}_D$ 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 $\mathcal{L}_D$.

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

$$\phi(x) := \lim_{\varepsilon\to 0} \int_{\{y\in\mathbb{R}^d : |y-x|>\varepsilon\}} (f(y) - f(x)) \frac{c_{d,\alpha}}{|y-x|^{d+\alpha}} dy \tag{4.7}$$

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

$$\begin{aligned} \mathcal{L}_D f(x) &= \lim_{\varepsilon\to 0} \int_{\{y\in\mathbb{R}^d : |y-x|>\varepsilon\}} (f(y) - f(x)) \frac{c_{d,\alpha}}{|y-x|^{d+\alpha}} dy \\ &= \int_{y\in\mathbb{R}^d} \left(f(x+y) - f(x) - \nabla f(x) \cdot y \mathbf{1}_{\{|y|\le 1\}} \right) \frac{c_{d,\alpha}}{|y|^{d+\alpha}} dy. \end{aligned}$$

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

$$\begin{aligned} \mathcal{E}^D(f, g) &= \frac{1}{2} \int_{\mathbb{R}^d\times\mathbb{R}^d} (f(x) - f(y))(g(x) - g(y)) \frac{c_{d,\alpha}}{|x-y|^{d+\alpha}} dxdy \\ &= \frac{1}{2} \lim_{\varepsilon\to 0} \int_{\{(x,y)\in\mathbb{R}^d\times\mathbb{R}^d : |x-y|>\varepsilon\}} (f(y) - f(x))(g(y) - g(x)) \frac{c_{d,\alpha}}{|y-x|^{d+\alpha}} dxdy \end{aligned}$$

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

Since $C_c^2(D)$ is $\mathcal{E}_1^D$-dense in $W_0^{\alpha/2,2}(D)$, this implies that $f\in \mathrm{Dom}(\mathcal{L}_D)$ 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

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

and the integral is a continuous function on D. Set

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

For any compact subset K of D, let

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

Defining

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

we have

$$\lim_{\varepsilon\to 0}\sup_{x\in K}\left|\int_{\{y\in\mathbb{R}^d:|y-x|>\varepsilon\}}(f(y)-f(x))\frac{c_{d,\alpha}}{|y-x|^{d+\alpha}}dy-\psi(x)\right|$$
$$=\lim_{\varepsilon\to 0}\sup_{x\in K}\left|\int_{\{y\in\mathbb{R}^d:|y-x|\le\varepsilon\}}\left(f(x+y)-f(x)-\nabla f(x)\cdot y\mathbf{1}_{\{|y|\le 1\}}\right)\frac{c_{d,\alpha}}{|y|^{d+\alpha}}dy\right|$$
$$\le\lim_{\varepsilon\to 0}\left|\int_{\{y\in\mathbb{R}^d:|y-x|\le\varepsilon\}}\sup_{z\in K_\varepsilon}\|D^2f\|_\infty\,|y|^2\,\frac{c_{d,\alpha}}{|y|^{d+\alpha}}dy\right|=0.$$

By what we have shown in the first part, this implies that $f\in\mathrm{Dom}(\mathcal{L}_D)$ 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:

$$\begin{aligned}&\frac{\partial^\beta}{\partial t^\beta}u(t,x)=\Delta^{\alpha/2}u(t,x);\quad x\in D,\ t>0\\&u(t,x)=0,\quad x\in D^c,\ t>0,\\&u(0,x)=f(x),\quad x\in D.\end{aligned}\tag{4.8}$$

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 $u(t,\cdot)\in W_0^{\alpha/2,2}(D)$ 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 $\psi\in C_c^1(0,\infty)$ and $\phi\in C_c^2(D)$,

$$\int_{\mathbb{R}^d}\left(\int_0^\infty u(t,x)\frac{\partial^\beta\psi(t)}{\partial t^\beta}dt\right)\phi(x)dx=\int_0^\infty \mathcal{E}^D(u(t,\cdot),\phi)\,\psi(t)\,dt.$$

(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 $\mathbb{P}_x[\tau_D(X)=0]=1$. 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. [18, 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 [18, 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 $L^2(D;dx)$: $P_t^D\psi_n=e^{-\lambda_n t}\psi_n$ in $C_\infty(D)$ (see [18, Theorem 3.3]). In particular, every eigenfunction ψ_n of the L^2-generator $\mathcal{L}_D$ is a bounded continuous function on D that vanishes continuously on the boundary ∂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 α-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 $f \in \mathrm{Dom}(\mathcal{L}_D^k)$ for some $k > -1 + (3d+4)/(2\alpha)$. Then*

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

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 $\mathcal{L}_D$ 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 $f \in \mathrm{Dom}(\mathcal{L}_D^k)$ for some $k > -1 + (3d+4)/(2\alpha)$, using (4.5) it follows that

$$M := \sum_{n=1}^{\infty} \lambda_n^{2k} \langle f, \psi_n \rangle^2 < \infty, \tag{5.1}$$

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

$$|\psi_n(x)| \leq c\lambda_n^{d/(2\alpha)} \quad \text{for every } x \in D \tag{5.2}$$

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 $f(x) = \sum_{n=1} \langle f, \psi_n\rangle \psi_n$ 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

$$\frac{\partial}{\partial t} v(t, x) = \Delta^{\alpha/2} v(t, x) \quad \text{with } v(0, x) = f(x) \tag{5.3}$$

on the Hilbert space $L^2(\mathbb{R}^d; dx)$ (cf. see [13]). 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 [19, Proposition 3.3], we have for every $j \geq 1$ and $1 \leq i \leq d$ that

$$\left|\frac{\partial^j}{\partial x_i^j} p(t, x, y)\right| \leq c\left(t^{-(d+j)/\alpha} \wedge \frac{t}{|x-y|^{d+\alpha+j}}\right) \leq c_1 t^{-j/\alpha} p(t, x, y). \tag{5.4}$$

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 $t \in (0, T]$,

$$\left|\frac{\partial^j}{\partial x_i^j} p_D(t, x, y)\right| \leq c_2 t^{-j/\alpha} p(t, x, y). \tag{5.5}$$

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) and (5.5), and the Cauchy–Schwarz inequality that

$$|\nabla^j P_t^D f(x)| \le c_3 t^{-j/\alpha}(2t)^{-d/(2\alpha)}\|f\|_{L^2(D)}. \tag{5.6}$$

Consequently, each eigenfunction $\psi_n(x) = e^{\lambda_n t} P_t^D \psi_n(x)$ is smooth inside D with

$$\left|\nabla^j \psi_n(x)\right| \le c_3 t^{-(d+2j)/(2\alpha)} e^{\lambda_n t}$$

for $x \in K$ and $t \in (0, T]$. Taking $t = 1/\lambda_n$ yields

$$\left|\nabla^j \psi_n(x)\right| \le c_3 \lambda_n^{(d+2j)/(2\alpha)} \quad \text{for } x \in K. \tag{5.7}$$

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^∞ 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

$$u(t,x) = \mathbb{E}_x[f(X^D_{E_t})] = \mathbb{E}_x[f(X_{E_t}); E_t < \tau_D].$$

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 Baeumer and Meerschaert [16, Theorem 3.1] (and [8, Theorem 4.2]), $u(t,x)$ is a weak solution for the parabolic equation (4.8) 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 [20] 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 $\mathbb{E}[e^{-\lambda E_t}] = E_\beta(-\lambda t^\beta)$. Then it follows, using (4.3) and a simple conditioning argument, that

$$\begin{aligned} u(t,x) &= \int_0^\infty \mathbb{E}_x\left[f(X_s); s < \tau_D\right] f_t(s)\,ds \\ &= \int_0^\infty \left(\sum_{n=1}^\infty e^{-s\lambda_n}\langle f,\psi_n\rangle\psi_n(x)\right) f_t(s)\,du \\ &= \sum_{n=1}^\infty E_\beta(-\lambda_n t^\beta)\langle f,\psi_n\rangle\psi_n(x). \end{aligned} \tag{5.8}$$

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

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

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

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

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 Krägeloh [21, Eq. (17)],

$$\left|\frac{\partial}{\partial t}E_\beta(-\lambda_n t^\beta)\right| \le c\frac{\lambda_n t^{\beta-1}}{1+\lambda_n t^\beta} \le c\,\lambda_n^\gamma\, t^{\gamma\beta-1}.$$

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

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

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

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

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 $f\in \mathrm{Dom}(\mathcal{L}_D^k)$ for some $k>1+(3d)/(2\alpha)$, then $u(t,x)=\mathbb{E}_x[f(X^D_{E_t})]$ 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 $\partial_t^\nu u=\Delta u$ on bounded domains. The distributed-order time-fractional derivative is defined by

$$\partial_t^\nu f(t)=\int \frac{\partial^\beta f(t)}{\partial t^\beta}\nu(d\beta),$$

where ν 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 $\partial_t^\nu u=\Delta^{\alpha/2}u$ 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 [23]. □

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 [6]. 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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