

SPACE–TIME DUALITY FOR FRACTIONAL DIFFUSION

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Abstract

Zolotarev (1961) proved a duality result that relates stable densities with different indices. In this paper we show how Zolotarev’s duality leads to some interesting results on fractional diffusion. Fractional diffusion equations employ fractional derivatives in place of the usual integer-order derivatives. They govern scaling limits of random walk models, with power-law jumps leading to fractional derivatives in space, and power-law waiting times between the jumps leading to fractional derivatives in time. The limit process is a stable Lévy motion that models the jumps, subordinated to an inverse stable process that models the waiting times. Using duality, we relate the density of a spectrally negative stable process with index $1 < \alpha < 2$ to the density of the hitting time of a stable subordinator with index $1/\alpha$, and thereby unify some recent results in the literature. These results provide a concrete interpretation of Zolotarev’s duality in terms of the fractional diffusion model. They also illuminate a current controversy in hydrology, regarding the appropriate use of space- and time-fractional derivatives to model contaminant transport in river flows.

Keywords: Limit theory; stable process; subordinator; fractional diffusion; duality

2000 Mathematics Subject Classification: Primary 60G52; 26A33

1. Introduction

A classical result of Zolotarev [51] (see also [25, Theorem 3.3]) equates stable densities with different indices. The proof of this result is purely analytical. In this paper we apply Zolotarev’s duality to prove some interesting results on fractional diffusion. Fractional derivatives are natural extensions of their integer-order analogues [35], [43]. Partial differential equations of fractional order are important in applications in physics [34], finance [45], and hydrology [6], [47]. In some cases, the solutions of the fractional equations govern the probability densities of certain heavy-tailed stochastic processes [27], [33], [39], [40]. This connection, a generalization of the link between Brownian motion and the diffusion equation [18], is very useful in both theoretical and applied work [8], [50]. Perhaps the simplest version of the fractional diffusion equation is $\partial^\gamma u / \partial t^\gamma = \partial^2 u / \partial x^2$ in one dimension, where the usual first derivative in time is replaced by the Caputo fractional derivative of order $0 < \gamma < 1$. Meerschaert *et al.* [27],

Received 14 April 2009; revision received 11 August 2009.

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Partially supported by NSF grants DMS-0803360 and EAR-0823965.

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[33] showed that the point source solution $u(x, t)$ to this equation gives the density of the stochastic process $B(E_t)$, where $B(x)$ is a Brownian motion and E_t is the inverse or hitting time of a stable subordinator with index γ . Orsingher and Beghin [39], [40] showed that the same solution can be written in terms of the normal density of $B(x)$ subordinated to a stable density with index $\alpha = 1/\gamma$. In this paper we reconcile these two results using Zolotarev’s duality. As a consequence, we reveal a concrete interpretation of the duality in terms of stable processes and their inverses. We also illustrate the modeling implications of our results, and clarify some recent empirical observations in river flow hydrology.

2. Duality

Stable laws are important because they represent the most general distributional limit for centered and normalized sums of independent and identically distributed (i.i.d.) random variables [20, Section XVII.5], [26, p. 321]. Since most stable densities cannot be written in closed form, it is common to use characteristic functions (Fourier transforms). A stable density $p(x)$ has characteristic function $\hat{p}(\lambda) = \int_{-\infty}^{\infty} e^{i\lambda x} p(x) dx$ and $p(x) = (1/2\pi) \int_{-\infty}^{\infty} e^{-i\lambda x} \hat{p}(\lambda) d\lambda$. Several different parameterizations of the family of stable densities are commonly used in the literature. One commonly used representation of the centered stable density is (see [25, Theorem 2.3])

$$p_{\alpha}(x; \theta, c) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i\lambda x} \exp\left\{-c|\lambda|^{\alpha} \left[1 + i\theta \frac{\lambda}{|\lambda|} \tan\left(\frac{\pi\alpha}{2}\right)\right]\right\} d\lambda, \tag{2.1}$$

where $c > 0$, $|\theta| \leq 1$, $0 < \alpha \leq 2$, and $\alpha \neq 1$.

A second parametrization is (see [20, p. 581] and [25])

$$p_{\alpha}(x; \eta, b) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i\lambda x} \exp\left\{-b|\lambda|^{\alpha} \exp\left\{-\frac{i\pi\eta}{2} \frac{\lambda}{|\lambda|}\right\}\right\} d\lambda, \quad \alpha \neq 1, \tag{2.2}$$

where $b > 0$ and η is real. The connection between (2.1) and (2.2) is as follows:

$$c = b \cos\left(\frac{\pi\eta}{2}\right) \quad \text{and} \quad \theta = -\cot\left(\frac{\pi\alpha}{2}\right) \tan\left(\frac{\pi\eta}{2}\right).$$

From the relation $|\theta| \leq 1$ we can conclude that $|\eta| \leq \alpha$ if $0 < \alpha < 1$, but $|\eta| \leq 2 - \alpha$ if $1 < \alpha \leq 2$.

Finally, the commonly used parametrization of Samorodnitsky and Taqqu [44, Definition 1.1.6] is

$$p_{\alpha}(x; \beta, \sigma) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i\lambda x} \exp\left\{-\sigma^{\alpha} |\lambda|^{\alpha} \left[1 - i\beta \frac{\lambda}{|\lambda|} \tan\left(\frac{\pi\alpha}{2}\right)\right]\right\} d\lambda, \quad \alpha \neq 1, \tag{2.3}$$

which is very similar to (2.1) except for a sign change. The scale parameter $\sigma > 0$ satisfies $c = \sigma^{\alpha}$ and the parameter $\beta = -\theta$ is called the skewness.

A duality result for stable densities was proved by Zolotarev [51] (see also [25]) using parametrization (2.2). The proof follows directly from the series representation for stable densities [25, Theorem 3.1].

Theorem 2.1. *If $1 < \alpha \leq 2$ then, for all $u > 0$, we have*

$$p_{\alpha}(u; \eta, 1) = u^{-(1+\alpha)} p_{\alpha^*}(u^{-\alpha}; \eta^*, 1), \tag{2.4}$$

where $\alpha^* = 1/\alpha$ and $\eta^* = (\eta - 1)/\alpha + 1$.

We will be interested in the case where the α -stable density on the left-hand side of (2.4) is totally negatively skewed ($\beta = -1$), which corresponds to $\theta = +1$ or, equivalently, $\eta = 2 - \alpha$. In this case, $\eta^* = \alpha^*$ and so the stable density on the right-hand side has $\theta^* = -1$, or in other words, its skewness is $\beta^* = +1$ (totally positively skewed). Then the right-hand side of (2.4) involves the density of a stable subordinator whose index $\gamma = \alpha^* = 1/\alpha$ satisfies $\frac{1}{2} \leq \gamma < 1$. After substituting back into (2.2), a little algebra shows that the characteristic function of the subordinator density is $\exp\{-(-i\lambda)^\gamma\}$.

3. Fractional diffusion

In applications to differential equations, the following parametrization of stable densities is useful (see [26, Remark 11.1.13]):

$$p_\alpha(x; q, a) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i\lambda x} \exp\{qa(i\lambda)^\alpha + (1 - q)a(-i\lambda)^\alpha\} d\lambda, \quad \alpha \neq 1,$$

which is related to (2.3) by $\beta = 1 - 2q$ and $\sigma^\alpha = -a \cos(\pi\alpha/2)$. Note that $0 \leq q \leq 1$, and $a > 0$ for $1 < \alpha < 2$, while $a < 0$ for $0 < \alpha < 1$. Let $A(t)$ be a stable Lévy process such that $A(t + s) - A(s)$ has density $p_\alpha(x; q, at)$, and is independent of $A(s)$. Define $d^\alpha p(x)/dx^\alpha$ to be the function with Fourier transform $(-i\lambda)^\alpha \hat{p}(\lambda)$, which extends the familiar formula for integer-order derivatives. Similarly, let $d^\alpha p(x)/d(-x)^\alpha$ be the function with Fourier transform $(i\lambda)^\alpha \hat{p}(\lambda)$. These are called the (positive and negative) Riemann–Liouville fractional derivatives. They can also be defined by

$$\frac{d^\alpha p(x)}{dx^\alpha} = \frac{1}{\Gamma(n - \alpha)} \frac{d^n}{dx^n} \int_{-\infty}^x \frac{p(\xi)}{(x - \xi)^{\alpha+1-n}} d\xi \tag{3.1}$$

and

$$\frac{d^\alpha p(x)}{d(-x)^\alpha} = \frac{(-1)^n}{\Gamma(n - \alpha)} \frac{d^n}{dx^n} \int_x^\infty \frac{p(\xi)}{(\xi - x)^{\alpha+1-n}} d\xi,$$

where n is an integer such that $n - 1 < \alpha \leq n$; see, for example [43]. Since

$$\hat{p}(\lambda, t) = \exp\{qat(i\lambda)^\alpha + (1 - q)at(-i\lambda)^\alpha\}$$

is evidently the solution to the ordinary differential equation

$$\frac{d}{dt} \hat{p}(\lambda, t) = \{qa(i\lambda)^\alpha + (1 - q)a(-i\lambda)^\alpha\} \hat{p}(\lambda, t)$$

with the point source initial condition $\hat{p}(\lambda, 0) \equiv 1$, we can invert the Fourier transform to see that the governing equation of the process $A(t)$ is

$$\frac{\partial p(x, t)}{\partial t} = qa \frac{\partial^\alpha p(x, t)}{\partial(-x)^\alpha} + (1 - q)a \frac{\partial^\alpha p(x, t)}{\partial x^\alpha}, \tag{3.2}$$

the space-fractional diffusion equation. Equation (3.2) originated in the work of Marcel Riesz [42] in the symmetric case, and was extended by Feller [19] to skewed stable laws, although fractional derivatives were not explicitly mentioned.

Let $D(t)$ be another stable Lévy process with index $0 < \gamma < 1$ and positive skewness (i.e. $\beta = 1$ in parameterization (2.3)). The governing equation for the density $f(x, t)$ of $D(t)$ is

$$\frac{\partial f(x, t)}{\partial t} = -b \frac{\partial^\gamma f(x, t)}{\partial x^\gamma},$$

where $b > 0$, and only the positive fractional derivative appears. Note that $f(x, t) = p_\gamma(x; \gamma, bt)$ in parametrization (2.2). Write $g_\gamma(x) = f(x, 1)$, and note that $D(ct) = c^{1/\gamma} D(t)$ in law (self-similarity). Define the inverse or hitting time process

$$E_t = \inf\{x > 0: D(x) > t\}, \tag{3.3}$$

and note that $\{D(x) > t\} = \{E_t < x\}$. Using the fact that $D(t)$ is self-similar, continuous in probability, and has a density, we see that E_t has cumulative distribution function

$$P(E_t \leq x) = P(D(x) \geq t) = P(x^{1/\gamma} D \geq t) = P\left(\left(\frac{D}{t}\right)^{-\gamma} \leq x\right).$$

Then it follows easily, by differentiating and using $f(x, t) = t^{-1/\gamma} g_\gamma(t^{-1/\gamma} x)$, that E_t has the density

$$h(x, t) = \frac{t}{\gamma} x^{-1-1/\gamma} g_\gamma(tx^{-1/\gamma}) \tag{3.4}$$

on $x > 0$ for all $t > 0$ (see [27, Corollary 3.1]).

The Laplace transform $\tilde{h}(x, s) = \int_0^\infty e^{-st} h(x, t) dt$ exists for all $x > 0$; see [28]. The Riemann–Liouville fractional derivative in time, $\partial^\gamma h(x, t)/\partial t^\gamma$, can be defined as the inverse Laplace transform of $s^\gamma \tilde{h}(x, s)$, or by the formula

$$\frac{\partial^\gamma h(x, t)}{\partial t^\gamma} = \frac{1}{\Gamma(1-\gamma)} \frac{\partial}{\partial t} \int_0^t \frac{h(x, \xi)}{(t-\xi)^\gamma} d\xi,$$

which agrees with definition (3.1) since $h(x, t) = 0$ for $t < 0$. Then a Laplace transform argument [28, Theorem 4.1] shows that

$$\frac{\partial h(x, t)}{\partial x} = -b \frac{\partial^\gamma h(x, t)}{\partial t^\gamma} + b\delta(x) \frac{t^{-\gamma}}{\Gamma(1-\gamma)}. \tag{3.5}$$

To briefly summarize the argument, note that $P(D(x) \leq t)$ has Laplace transform $s^{-1} e^{-xbs^\gamma}$, so that $h(x, t) = d[1 - P(D(x) \leq t)]/dx$ has Laplace transform $bs^{\gamma-1} e^{-xbs^\gamma}$. Take Laplace transforms in the other variable x to see that

$$\bar{h}(\lambda, s) = \int_0^\infty \int_0^\infty e^{-\lambda x} e^{-st} h(x, t) dt dx = \frac{bs^{\gamma-1}}{\lambda + bs^\gamma},$$

and rearrange to obtain $\lambda \bar{h}(\lambda, s) = -bs^\gamma \bar{h}(\lambda, s) + bs^{\gamma-1}$, which is the double Laplace transform of (3.5), since $s^{\gamma-1}$ is the Laplace transform of $t^{-\gamma}/\Gamma(1-\gamma)$.

A simple conditioning argument shows that $A(E_t)$ has density

$$m(x, t) = \int_0^\infty p(x, u) h(u, t) du. \tag{3.6}$$

Similar to (3.5), an argument with Fourier and Laplace transforms [28, Theorem 4.1] shows that the overall governing equation is

$$b \frac{\partial^\gamma m(x, t)}{\partial t^\gamma} = qa \frac{\partial^\alpha m(x, t)}{\partial (-x)^\alpha} + (1-q)a \frac{\partial^\alpha m(x, t)}{\partial x^\alpha} + b\delta(x) \frac{t^{-\gamma}}{\Gamma(1-\gamma)}, \tag{3.7}$$

using the appropriate Riemann–Liouville fractional derivatives on both sides.

Remark 3.1. The Caputo fractional derivative

$$\left(\frac{\partial}{\partial t}\right)^\gamma F(t) = \frac{1}{\Gamma(1-\gamma)} \int_0^t \frac{dF(\xi)/d\xi}{(t-\xi)^\gamma} d\xi \tag{3.8}$$

for $0 < \gamma \leq 1$ is the inverse Laplace transform of $s^\gamma \tilde{F}(s) - s^{\gamma-1} F(0)$; see, for example, [13] and [41, pp. 79–80]. This extends the usual integer-order formula, and is useful in differential equations, since it includes the initial value. Then we can write (3.7) more compactly in the form

$$b\left(\frac{\partial}{\partial t}\right)^\gamma m(x, t) = qa \frac{\partial^\alpha m(x, t)}{\partial(-x)^\alpha} + (1-q)a \frac{\partial^\alpha m(x, t)}{\partial x^\alpha}. \tag{3.9}$$

Similarly, we can rewrite (3.5) in the form

$$b\left(\frac{\partial}{\partial t}\right)^\gamma h(x, t) = -\frac{\partial h(x, t)}{\partial x}, \tag{3.10}$$

which can be considered a degenerate case of (3.9) with $A(u) = u$. See [28] for more details and complete proofs.

Remark 3.2. Chaves [15] pioneered the use of (3.2) to model anomalous diffusion in physics. Anomalous diffusion occurs when the long-time limit of diffusing particles deviates from Brownian motion. The random walk $S(n) = Y_1 + \dots + Y_n$ represents a particle location after n jumps. Suppose that Y_n belongs to the domain of attraction of some stable random variable A with index $0 < \alpha \leq 2$, and assume for simplicity that $n^{-1/\alpha} S_n \Rightarrow A$. (In the general case, we can replace the norming constants $n^{-1/\alpha}$ by a regularly varying sequence with index $-1/\alpha$; see, for example, [20, XVII.5].) Then the random walk scaling limit is $c^{-1/\alpha} S_{[ct]} \Rightarrow A(t)$, a stable Lévy process with index α . The limit is self-similar with $A(ct) = c^{1/\alpha} A(t)$ in distribution, so that, for $\alpha < 2$, the spreading rate is faster than Brownian motion (the special case $\alpha = 2$). In physics, this is called anomalous super-diffusion. Then $A(t)$ satisfies a tail condition $P(|A(t)| > x) \sim Ctx^{-\alpha}$, where $C = -a/\Gamma(1-\alpha)$ for $0 < \alpha < 1$ and $C = a(\alpha-1)/\Gamma(2-\alpha)$ for $1 < \alpha < 2$ [44, Proposition 1.2.15]. Thus, the order of the fractional derivative in (3.2) equals the tail index of the stable law. In addition, the weak convergence $n^{-1/\alpha} S_n \Rightarrow A$ requires $P(|Y_n| > x) \sim Cx^{-\alpha}$ for large x , so the order of the fractional derivative also reflects the tail behavior of particle jumps. Finally, note that $P(Y_n < -x)/P(|Y_n| > x) \rightarrow q$ as $x \rightarrow \infty$, so that the positive and negative fractional derivatives in the governing equation (3.2) reflect the positive and negative tails of particle jumps.

Space–time fractional diffusion equations are the governing equations of certain stochastic processes that occur as scaling limits of continuous-time random walks [27], [33]. A continuous-time random walk (CTRW) is simply a random walk in which the i.i.d. jumps (Y_n) are separated by i.i.d. random waiting times (J_n). The CTRW was developed as a model in statistical physics [36], [46]. A random particle jump Y_n follows a random waiting time $J_n > 0$. The random walk $S(n) = Y_1 + \dots + Y_n$ gives the particle location after n jumps. Another random walk $T(n) = J_1 + \dots + J_n$ gives the time of the n th jump. The number of jumps by time $t > 0$ is given by the renewal process $N_t = \max\{n \geq 0: T(n) \leq t\}$. The location of a particle at time $t > 0$ is $S(N_t)$, a random walk subordinated to a renewal process. The long-time behavior of particles is described by a limit theorem [27]. Suppose that $P(J_n > t) = t^{-\gamma} L_1(t)$ for some $0 < \gamma < 1$, where L_1 is slowly varying. Then T_n belongs to the domain of attraction

of some stable law with index γ . To simplify the exposition, consider the special case where $L_1(t) \rightarrow C > 0$ is asymptotically constant as $t \rightarrow \infty$. Then $n^{-1/\gamma}T_n \Rightarrow D$ as $n \rightarrow \infty$, where D is a stable random variable with index γ . Suppose also that Y_n belongs to the domain of attraction of some stable random variable A with index $0 < \alpha \leq 2$ and that $n^{-1/\alpha}S_n \Rightarrow A$. Restricting to the uncoupled case where Y_n and J_n are independent (see [5] for the coupled case) we can extend to process convergence, $c^{-1/\gamma}T_{[ct]} \Rightarrow D(t)$ and $c^{-1/\alpha}S_{[ct]} \Rightarrow A(t)$, where $A(t)$ and $D(t)$ are independent Lévy stable processes with $A(1) = A$ and $D(1) = D$ in distribution, and the convergence is in terms of all finite-dimensional distributions (or the appropriate Skorokhod topology; see [27]). Continuous mapping arguments [27] lead to $c^{-\gamma}N_{[ct]} \Rightarrow E_t$, and then $c^{-\gamma/\alpha}S(N_{[ct]}) \Rightarrow A(E_t)$.

4. Space–time duality

Here we apply Zolotarev’s duality from Section 2 to the space–time fractional diffusion equation from Section 3. The following result uses parametrization (2.2). Recall that a stable subordinator is a stable Lévy process with nondecreasing sample paths. This requires index $\alpha < 1$ and positive skewness; see, for example, [7, p. 71]. In the following, when we say that E_t is identically distributed with $Y(t) \mid Y(t) > 0$, we mean that the distribution of $E(t)$ is the same as the conditional distribution of $Y(t)$ given $Y(t) > 0$.

Theorem 4.1. *Let $D(t)$ be a stable subordinator with density $p_\gamma(x; \gamma, bt)$ for some $\frac{1}{2} \leq \gamma < 1$. Let E_t be the hitting time (3.3) with density (3.4), where $g_\gamma(x) = p_\gamma(x; \gamma, b)$ is the density of $D(1)$, and let $Y(t)$ denote a stable Lévy motion with density $p_\alpha(x; 2 - \alpha, b^{-\alpha}t)$, where $\alpha = 1/\gamma$. Then*

- (i) $P(Y(t) > 0) = 1/\alpha$ for all $t > 0$,
- (ii) E_t is identically distributed with $Y(t) \mid Y(t) > 0$ for each $t > 0$.

Proof. Using the self-similarity property $p_\alpha(u; \eta, b) = b^{-1/\alpha} p_\alpha(b^{-1/\alpha}u; \eta, 1)$ for stable densities, the density of $Y(t)$ for $t > 0$ is

$$P(x, t) = bt^{-1/\alpha} p_\alpha(bt^{-1/\alpha}x; \eta, 1).$$

Apply (2.4) with $u = bt^{-1/\alpha}x$ and $\eta = 2 - \alpha$ to see that

$$P(x, t) = bt^{-1/\alpha} u^{-1-\alpha} p_{\alpha^*}(u^{-\alpha}; \eta^*, 1)$$

for $x > 0$, where $\alpha^* = 1/\alpha = \gamma$ and $\eta^* = \alpha^{-1}(\eta - 1) + 1 = \gamma$. Simplify to obtain

$$P(x, t) = tx^{-1-1/\gamma} b^{-1/\gamma} p_\gamma(b^{-1/\gamma}tx^{-1/\gamma}; \gamma, 1)$$

and recall that $g_\gamma(x) = p_\gamma(x; \gamma, b) = b^{-1/\gamma} p_\gamma(b^{-1/\gamma}x; \gamma, 1)$ is the density of $D(1)$. Then

$$P(x, t) = tx^{-1-1/\gamma} g_\gamma(tx^{-1/\gamma}) \quad \text{for } x > 0.$$

Compare with (3.4) to conclude that

$$P(x, t) = \gamma h(x, t) \tag{4.1}$$

for $t > 0$ and $x > 0$. Since $\int_0^\infty h(x, t) dx = 1$ for all $t > 0$, we have $P(Y(t) > 0) = \gamma = 1/\alpha$ for all $t > 0$. Thus, the density of E_t equals the conditional density of $Y(t)$ given $Y(t) > 0$ for all $t > 0$.

Remark 4.1. As the scaling limit of a random walk with positive jumps, the stable subordinator $D(t)$ is totally positively skewed with $\beta = 1$ in (2.3). The process $Y(t)$ has skewness $\beta = -1$, so it is the scaling limit of a random walk with only negative jumps. This is also called a spectrally negative process, since the Lévy measure assigns no mass to the positive real line. Bingham [10] pointed out that the hitting time $D(t) = \inf\{u : Y(u) > t\}$ is a stable subordinator with index $1/\alpha$ and that there is a version of $Y(t)$ for which $Y(D(t)) \equiv t$. Hence, $D(t)$ is the process inverse of $Y(t)$, but E_t is the process inverse of $D(t)$. Thus, the inverse of the inverse of $Y(t)$ is the process E_t , whose one-dimensional distributions are the same as those of $Y(t) \mid Y(t) > 0$. Note that $D(E_t) > t$ almost surely since $D(t)$ is a pure-jump process [7, p. 77]. If $\alpha = 2$ then $Y(t)$ is a Brownian motion, and the skewness is irrelevant.

Remark 4.2. Using the series representation for stable densities [25, Theorem 3.1], it is not hard to prove Theorem 4.1 directly. For convenience, we consider $b = t = 1$; the remaining cases follow easily by self-similarity. Then the density of $Y(1)$ for $x > 0$ is

$$p_\alpha(x; \eta, 1) = \frac{1}{\pi} \sum_{k=1}^\infty (-1)^{k+1} \frac{\Gamma(1 + k/\alpha)}{k!} x^{k-1} \sin\left(\frac{\pi k(\eta + \alpha)}{2\alpha}\right),$$

where $\eta = 2 - \alpha$. The density of stable subordinator D is

$$g_\gamma(x) = \frac{1}{\pi} \sum_{k=1}^\infty (-1)^{k+1} \frac{\Gamma(\gamma k + 1)}{k!} x^{-\gamma k - 1} \sin(\pi k \gamma).$$

Then the density of E_1 is

$$\begin{aligned} x^{-1-\alpha} g_\gamma(x^{-\alpha}) &= \alpha \frac{x^{-1-\alpha}}{\pi} \sum_{k=1}^\infty (-1)^{k+1} \frac{\Gamma(1 + k/\alpha)}{k!} x^{-(k/\alpha - 1)(-\alpha)} \sin\left(\frac{\pi k}{\alpha}\right) \\ &= \alpha \frac{1}{\pi} \sum_{k=1}^\infty (-1)^{k+1} \frac{\Gamma(1 + k/\alpha)}{k!} x^{k-1} \sin\left(\frac{\pi k}{\alpha}\right) \\ &= \alpha p_\alpha(x; (2 - \alpha), 1). \end{aligned}$$

Theorem 4.1 has some immediate consequences for space–time diffusion equations. The discussion in Section 3 explains how space-fractional derivatives model heavy-tailed power-law particle jumps, and time-fractional derivatives model power-law waiting times. The duality theorem, Theorem 4.1, connects heavy-tailed jumps with fractional time derivatives, and conversely, it relates heavy-tailed waiting times to fractional derivatives in space.

The Caputo fractional derivative (3.8) was used in the governing equation (3.10). Then the next result follows immediately from (4.1).

Corollary 4.1. *Let $Y(t)$ denote a stable Lévy motion with index $1 < \alpha \leq 2$ and density $P(x, t) = p_\alpha(x; 2 - \alpha, b^{-\alpha}t)$ in parametrization (2.2). Then*

$$b\left(\frac{\partial}{\partial t}\right)^\gamma P(x, t) = -\frac{\partial P(x, t)}{\partial x}$$

holds for all $t > 0$ and $x > 0$.

The process $Y(t)$ is totally negatively skewed, so its density $P(x, t)$ solves a space-fractional equation similar to (3.2) with $q = 1$, using a negative Riemann–Liouville fractional derivative

$$\frac{\partial^\alpha P(x, t)}{\partial(-x)^\alpha} = \frac{1}{\Gamma(2 - \alpha)} \frac{d^2}{dx^2} \int_x^\infty \frac{P(y, t)}{(y - x)^{\alpha-1}} dy \tag{4.2}$$

with $1 < \alpha < 2$. In general, the α -order negative Riemann–Liouville fractional derivative is defined as the n th derivative of a fractional integral of order $n - \alpha$, where $n - 1 < \alpha < n$ [43].

Corollary 4.2. *Let $D(1)$ be a stable subordinator with density $g_\gamma(x) = p_\gamma(x; \gamma, b)$ in parametrization (2.2). Let E_t denote the hitting time process defined by (3.3). Then the density $h(x, t)$ of E_t solves*

$$\frac{\partial h(x, t)}{\partial t} = b^{-\alpha} \frac{\partial^\alpha h(x, t)}{\partial(-x)^\alpha} \tag{4.3}$$

for all $t > 0$ and $x > 0$.

Proof. A comparison with (3.2) shows that the density $P(x, t)$ of $Y(t)$ solves the space-fractional diffusion equation

$$\frac{\partial P(x, t)}{\partial t} = b^{-\alpha} \frac{\partial^\alpha P(x, t)}{\partial(-x)^\alpha}, \tag{4.4}$$

where we note that $c = \sigma^\alpha = -a \cos(\pi\alpha/2) = b^{-\alpha} \cos(\pi(2 - \alpha)/2)$. Then (4.3) follows using (4.1) and the fact that the negative fractional derivative in (4.4) depends only on $P(y, t)$ for $y > x$.

Remark 4.3. The characteristic function (Fourier transform) of $P(x, t)$ is

$$\hat{P}(\lambda, t) = \exp(tb^{-\alpha}(i\lambda)^\alpha).$$

It is common to analyze partial differential equations like (4.4) using transforms. Note, however, that the Fourier transform of $P(x, t) \mathbf{1}(x > 0)$ is not equal to $\hat{P}(\lambda, t)$ since $P(x, t)$ is supported on the entire real line. Since we restrict to the positive reals, it is convenient to use Laplace transforms. Bingham [9] and Bondesson *et al.* [11] showed that

$$\int_0^\infty e^{-zx} h(x, t) dx = E_\gamma(-zb^{-1}t^\gamma)$$

in terms of the Mittag–Leffler function

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

Then it follows from (4.1) that

$$\int_{-\infty}^\infty e^{-zx} P(x, t) \mathbf{1}(x > 0) dx = \gamma E_\gamma(-zb^{-1}t^\gamma),$$

which shows that the conditional distribution of $Y(t) \mid Y(t) > 0$ is Mittag–Leffler.

For an \mathbb{R}^d -valued Markov process $X(t)$, the family of linear operators

$$T(t)r(x) = E_x[r(X(t))] = E[r(X(t)) \mid X(0) = x]$$

forms a bounded continuous semigroup on the Banach space $L^1(\mathbb{R}^d)$, and the generator $L_x r(x) = \lim_{h \downarrow 0} h^{-1}(T(h)r(x) - r(x))$ is defined on a dense subset of that space [2, p. 110], [21, p. 648]. Then $p(x, t) = T(t)r(x)$ solves the abstract Cauchy problem defined as

$$\frac{\partial}{\partial t} p(x, t) = L_x p(x, t), \quad p(x, 0) = r(x), \tag{4.5}$$

for $t > 0$ and $x \in \mathbb{R}^d$. Nigmatullin [37] considered an abstract time-fractional Cauchy problem:

$$\left(\frac{\partial}{\partial t}\right)^\gamma m(x, t) = L_x m(x, t), \quad m(0, x) = r(x), \tag{4.6}$$

which reduces to (3.9) in the special case where $X(t)$ is a stable Lévy process started at $x = 0$. Zaslavsky [48] used (4.6) to model Hamiltonian chaos. Baeumer and Meerschaert [3] and Meerschaert and Scheffler [27] showed that the solution to (4.6) can be written in the form (3.6), where $h(x, t)$ is the density of E_t , the hitting time (3.3) of a standard stable subordinator $D(t)$, and $g_\gamma(x) = p_\gamma(x; \gamma, 1)$ is the density of $D(1)$. It follows easily that $m(x, t) = E_x[r(X(E(t)))]$. Then the next result follows immediately using (4.1).

Lemma 4.1. *Let $Y(t)$ denote a totally negatively skewed stable Lévy motion with index $1 < \alpha \leq 2$ and density $p_\alpha(x; 2-\alpha, t)$ in parametrization (2.2). Then the abstract fractional Cauchy problem (4.6) with $\gamma = 1/\alpha$ can be solved by taking $m(x, t) = E_x[r(X(Y(t)))] \mid Y(t) > 0$.*

Next we come to the problem that motivated this paper. For $\frac{1}{2} \leq \gamma < 1$, Orsingher and Beghin [40, Equation (5.23)] showed that the fractional Cauchy problem (4.5) in dimension $d = 1$ with $L_x = \partial^2/\partial x^2$ has solution

$$m(x, t) = \frac{1}{\gamma} \int_0^\infty p(x, u) p_{1/\gamma}\left(u, \frac{1}{\gamma}(2\gamma - 1), t\right) du, \tag{4.7}$$

using parametrization (2.2), where

$$p(x, u) = T(u)r(x) = \int_{\mathbb{R}} \frac{e^{-(x-y)^2/4u}}{\sqrt{4\pi u}} r(y) dy$$

is the heat semigroup corresponding to Brownian motion in \mathbb{R} . Note that (4.7) involves a stable density, while the equivalent solution, (3.6), replaces this by an inverse stable density. The next result shows how to equate these two forms. It also extends the result of [40] to an abstract fractional Cauchy problem on \mathbb{R}^d .

Theorem 4.2. *For $\frac{1}{2} \leq \gamma < 1$, the abstract fractional Cauchy problem (4.6) associated with the Markov process $X(t)$ has two equivalent solutions:*

$$\begin{aligned} m(x, t) &= E_x[r(X(E_t))] \\ &= \frac{t}{\gamma} \int_0^\infty p(x, u) g_\gamma\left(\frac{t}{u^{1/\gamma}}\right) u^{-1/\gamma-1} du \\ &= E_x[r(X(Y(t)))] \mid Y(t) > 0 \\ &= \frac{1}{\gamma} \int_0^\infty p(x, u) p_{1/\gamma}\left(u, \frac{1}{\gamma}(2\gamma - 1), t\right) du, \end{aligned} \tag{4.8}$$

where $p(x, t) = E_x[r(X(t))]$ solves the abstract Cauchy problem (4.5), E_t is the hitting time

(3.3) of a standard stable subordinator $D(t)$, $g_\gamma(x) = p_\gamma(x; \gamma, 1)$ is the density of $D(1)$, and $Y(t)$ is a totally negatively skewed stable Lévy motion with index $\alpha = 1/\gamma$ and density $p_\alpha(x; 2 - \alpha, t)$ in parametrization (2.2).

Proof. The integral solution on the second line of (4.8) was proven in [27, Theorem 5.1], and then the representation $E_x[r(X(E_t))]$ follows from (3.4). This also shows that the integral on the second line of (4.8) reduces to (3.6). Now the last line of (4.8) follows from Lemma 4.1 together with Theorem 4.1.

Remark 4.4. The skewed stable density in the fractional Cauchy problem solution (4.7) is supported on the entire real line, but the integral is over the positive reals. Orsingher and Beghin [40] commented that the solution, in dimension $d = 1$ with $L_x = \partial^2/\partial x^2$, can be expressed as $E_x[r(B(|Y(t)|))]$, where $B(t)$ is a standard Brownian motion and $Y(t)$ is the stable process from Theorem 4.2, so that $u = |Y(t)|$ has the density

$$Q(u, t) = \frac{1}{\gamma} p_{1/\gamma}\left(|u|, \frac{1}{\gamma}(2\gamma - 1), t\right).$$

This statement is correct in the case $\gamma = \frac{1}{2}$; see also [4]. However, for $\frac{1}{2} < \gamma < 1$, the restriction of the skewed stable density to the positive reals is not equivalent to a simple folding. Hence, the comment in that paper requires a small adjustment.

Meerschaert *et al.* [32] showed that, under some technical conditions, the abstract fractional Cauchy problem (4.6) with $0 < \gamma < 1$ in a bounded domain $D \subset \mathbb{R}^d$ with Dirichlet boundary conditions $m(x, 0) = r(x)$ for $x \in D$ and $m(x, t) = 0$ for $x \in \partial D$ and $t > 0$ is solved by taking

$$m(x, t) = E_x[r(X(E_t)) \mathbf{1}(\tau(X) > E_t)] = \int_0^\infty p(x, u)h(u, t) du, \tag{4.9}$$

where $\tau(X) = \inf\{t \geq 0: X_t \notin D\}$ is the first exit time, the generator L_x of the semigroup $T(t)f(x) = E_x[f(X_t) \mathbf{1}(\tau(X)) > t]$ is a uniformly elliptic operator of divergence form, $p(x, t) = T(t)r(x)$, E_t is the hitting time (3.3) of the standard stable subordinator, and $h(x, t)$ is the density of E_t as given by (3.4). Then the next result, which extends Theorem 4.2 to bounded domains, follows immediately from (4.1).

Theorem 4.3. *Under the technical conditions of [32, Theorem 3.6], the abstract fractional Cauchy problem (4.6) with $\frac{1}{2} \leq \gamma < 1$ in a bounded domain $D \subset \mathbb{R}^d$ with Dirichlet boundary conditions $m(x, 0) = r(x)$ for $x \in D$ and $m(x, t) = 0$ for $x \in \partial D$ and $t > 0$ has a unique classical solution*

$$\begin{aligned} m(x, t) &= E_x[r(X(Y(t))) \mathbf{1}(\tau(X) > Y(t)) \mid Y(t) > 0] \\ &= \alpha \int_0^\infty p(x, u)p_\alpha(u, (2 - \alpha), t) du \end{aligned} \tag{4.10}$$

with $\tau(X)$, L_x , and $p(x, t)$ as in the preceding paragraph, E_t is the hitting time (3.3) of a standard stable subordinator $D(t)$, $g_\gamma(x) = p_\gamma(x; \gamma, 1)$ is the density of $D(1)$, and $Y(t)$ is a totally negatively skewed stable Lévy motion with index $\alpha = 1/\gamma$ and density $p_\alpha(x; 2 - \alpha, t)$ in parametrization (2.2).

Remark 4.5. The space–time duality results in this paper help to clarify a current controversy in river flow hydrology. As explained in Remark 3.2, space-fractional derivatives model long jumps, and time-fractional derivatives model long waiting times, due to the underlying random

walk model. In applications to water pollution, the movement of contaminated particles is represented by this random walk. Long jumps occur when the particle enters a zone of high water velocity. Long waiting times between jumps occur when a particle is stuck in an eddy, or buried in a stream bed. Recently, it has been observed that the movement of contaminated particles in a river flow can be accurately modeled using a stable Lévy motion with negative skewness and tail index $1 < \alpha < 2$; see [17], [22], and [23]. Kim and Kavvas [24] contended that the negative skewness is due to particle waiting times. Zhang *et al.* [49] argued that, since a negative fractional derivative in space derives from large negative (upstream) jumps in the underlying random walk model, a negatively skewed model for transport in river flows is not physically meaningful. They argued that particle waiting times should be modeled using a fractional derivative in time, consistent with the random walk limit in Remark 3.2. The results of this paper suggest one possible reason why a negatively skewed stable could fit experimental data so well, even though a river cannot transport particles large distances upstream. Since the density of a negatively skewed stable with index $\alpha > 1$, restricted to the positive real line, equals the density of the inverse stable with index $1/\alpha < 1$, the time-fractional model in [49] and the space-fractional model in [17], [22], [23], and [24] are mathematically equivalent, under some conditions. Physically, we can understand that whether a particle jumps upstream, or whether it remains motionless while the bulk of the plume moves downstream, it ends up behind the center of mass. Hence, while the physical meaning of the time-fractional model is more natural, the space-fractional model is also reasonable. For additional details, see [14].

5. Remarks on simulation

Recall that the probability density $h(x, t)$ of the inverse stable subordinator E_t defined by (3.3) solves a time-fractional diffusion equation (3.10). A simple numerical solution method for (3.10) is to simulate a large number of replications of the process E_t and histogram the results. This method is known as particle tracking [50], also called the Lagrangian method. An alternative Eulerian method is based on a finite difference approximation of the fractional derivative [29]. In this section we will examine the implications of space–time duality for both Lagrangian and Eulerian simulations. Corollary 4.2 shows that $h(x, t)$ also solves the space-fractional partial differential equation (4.3) for all $t > 0$ and $x > 0$. Generally, space-fractional equations are simpler to simulate. Lack of memory in time permits efficient Lagrangian simulation based on the underlying Markov process. The same lack of memory allows Eulerian methods to efficiently step through time. Since a wide variety of time-fractional partial differential equations can be solved via subordination to the E_t process, the results discussed here have broad applicability.

The space-fractional diffusion equation (4.3) is under-specified, since we desire solutions on $x > 0$, and the equivalent equation, (4.4), has another solution $P(x, t)$ supported on the entire real line. To obtain a unique solution, we impose a suitable boundary condition. Let $D(1)$ be a stable subordinator with density $g_\gamma(x) = p_\gamma(x; \gamma, b)$ in parametrization (2.2). Let E_t denote the hitting time process defined by (3.3). Then the density $h(x, t)$ of E_t solves the boundary value problem

$$\frac{\partial h(x, t)}{\partial t} = b^{-\alpha} \frac{\partial^\alpha h(x, t)}{\partial(-x)^\alpha}, \quad \frac{\partial^{\alpha-1}}{\partial(-x)^{\alpha-1}} h(0, t) = 0. \quad (5.1)$$

To see this, note first that Theorem 4.1(i) shows that the total mass assigned to the positive real

line is $\int_0^\infty P(x, t) dx = 1/\alpha$, which remains fixed for all $t > 0$. Hence,

$$0 = \frac{\partial}{\partial t} \int_0^\infty P(x, t) dx = \int_0^\infty \frac{\partial^\alpha}{\partial(-x)^\alpha} P(x, t) dx = \frac{\partial^{\alpha-1}}{\partial(-x)^{\alpha-1}} P(0, t) \tag{5.2}$$

for all $t > 0$. Recall from (4.2) that the fractional derivative $\partial^\alpha/\partial(-x)^\alpha P(x, t)$ is defined for $1 < \alpha < 2$ as the second derivative of the fractional integral of order $2-\alpha$. Then the last equality in (5.2) follows from the fundamental theorem of calculus and the fact that $\partial^\alpha/\partial(-x)^\alpha P(x, t)$ is defined as the first derivative of that same fractional integral, up to a change of sign. Then (5.1) follows from (4.1).

Now the hitting time density $h(x, t)$ can be computed as the point source solution to the space-fractional boundary value problem (5.1). Discretize in space $x_i = i \Delta x$ and time $t_j = j \Delta t$ using the shifted Grünwald finite difference approximation [30]:

$$\frac{\partial^\alpha h(x, t)}{\partial(-x)^\alpha} = \lim_{\Delta x \rightarrow 0} (\Delta x)^{-\alpha} \sum_{n=0}^\infty (-1)^n \binom{\alpha}{n} h(x + (n-1)\Delta x, t),$$

where the fractional Binomial coefficients are defined by

$$\binom{\alpha}{n} = \frac{\Gamma(\alpha + 1)}{\Gamma(\alpha - n + 1)\Gamma(n + 1)}.$$

Then we approximate $h_{ij} = h(x_i, t_j)$ using an explicit Euler scheme:

$$\frac{h_{ij} - h_{i,j-1}}{\Delta t} = (b\Delta x)^{-\alpha} \sum_{n=0}^\infty (-1)^n \binom{\alpha}{n} h_{i+n-1,j-1},$$

which reduces to a stable recursive equation for h_{ij} , except at the boundary $i = 0$ where we apply the boundary condition

$$h_{0j} = - \sum_{n=1}^\infty (-1)^n \binom{\alpha - 1}{n} h_{i+n-1,j},$$

using the shifted Grünwald approximation once more. The effect of the boundary condition is to capture the mass that would have exited to the left, into the negative real line, and keep it at $x = 0$ to preserve mass. Figure 1 shows the results of solving boundary value problem (5.1) in the case $b = 1$ via this explicit Euler method. Figure 1 also shows a semi-analytical solution using (3.4), where the stable density g_γ was approximated using the algorithm of Nolan [38]. Richardson extrapolation is based on the fact that the error in the explicit Euler method is approximately proportional to the step size Δx . Therefore, a useful estimate of the error at step size Δx is $h_{ij}^{2\Delta x} - h_{ij}^{\Delta x}$, and the extrapolated curve is simply the numerical solution at $\Delta x = 0.2$ minus this approximate error.

An alternative Lagrangian approach is to simulate the Markov process $t_i = D(x_i)$ at times $x_i = i \Delta x$ as a sum of i.i.d. stable random variables with density $g_\gamma(t) = p_\gamma(t; \gamma, b\Delta x)$. Then we can approximate the inverse process $x_i = E(t_i)$ (at unequally spaced points) and linearly interpolate in t . A histogram of $E(t)$ values from a large number of iterations can be used to approximate the density $h(x, t)$, and more generally, to solve time-fractional diffusion equations via subordination [50]. An alternative Lagrangian method that requires no interpolation uses the

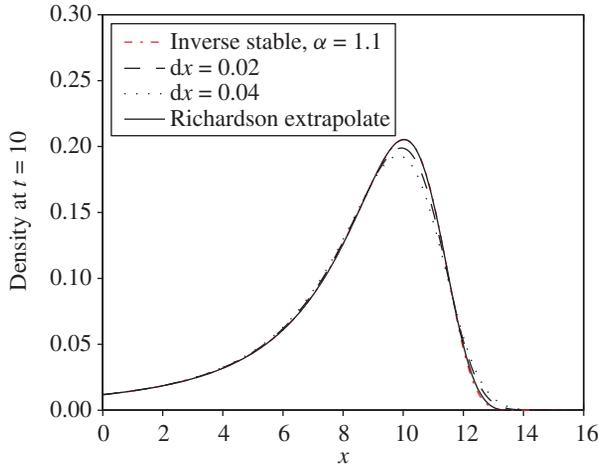


FIGURE 1: Extrapolated Eulerian solution to the boundary value problem (5.1) matches the inverse stable density $h(x, t)$ from (3.4).

space–time duality from Theorem 4.1. Since $E(t)$ is identically distributed with $Y(t) \mid Y(t) > 0$, we need only simulate the Markov process $Y(t)$ and approximate the conditional density via the histogram. Note that the proportion of sample paths with $Y(t) > 0$ will remain approximately constant since $P(Y(t) > 0) = 1/\alpha$ for all $t > 0$. Hence, this Lagrangian approach is reasonably efficient.

Remark 5.1. It is also interesting to find a stochastic process $Z(t)$ whose one-dimensional distributions are the same as the conditional distributions of $Y(t) \mid Y(t) > 0$, since the process $Z(t)$ could be used directly as a subordinator to solve time-fractional diffusion equations. For $\alpha = 2$, we can certainly take $Z(t) = |Y(t)|$ by the reflection principle. This fact is used, for example, to show that iterated Brownian motion $B(Y(t))$ [12] and Brownian motion in Brownian time $B(|Y(t)|)$ [1], [16] have the same one-dimensional distributions, and, hence, the same governing equation. For $1 < \alpha < 2$, the process $Y(t)$ is not symmetric, and the reflection principle does not apply. One possible alternative is to define $Z(t) = Y(u)$, where $u = u(t)$ is the process inverse of

$$t = t(u) = \int_0^u \mathbf{1}(Y(s) > 0) \, ds,$$

so that $t(u)$ is the length of time $Y(s)$ spends being positive during $0 < s < u$. Note that, generally, $t \leq u$, so that $u = u(t) \geq t$. In other words, take a sample path of $Y(t)$, snip out the parts where $Y(t) \leq 0$, and glue the remaining parts back together without any gaps in time. Figure 2 compares the results of a particle tracking simulation for this process with the density $h(x, t)$, computed semi-analytically using (3.4), as in Figure 1. In this figure, $b = 1$, $\alpha = 1.1$, $n = 2 \times 10^5$ particles were simulated, and a time step of $\Delta t = 0.05$ was used in the random walk approximation of $Y(t)$. The excellent agreement is encouraging.

The process $Z(t)$ is related to local times [7, p. 104]. The occupation measure

$$\mu_t(B) = \int_0^t \mathbf{1}(Y(s) \in B) \, ds$$

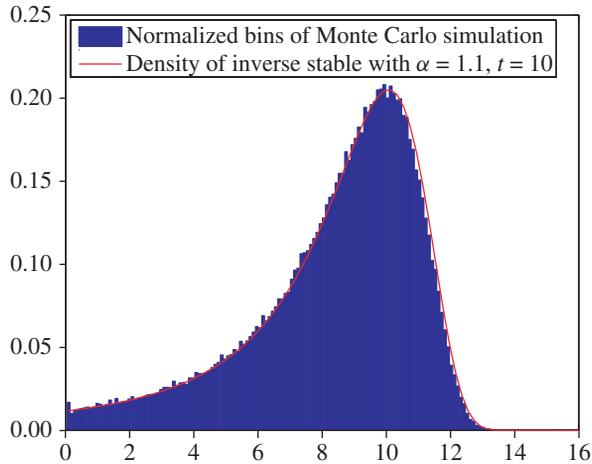


FIGURE 2: Particle tracking simulation of $Z(t)$ matches the conditional density of $Y(t) \mid Y(t) > 0$.

is well defined for the stable process $Y(t)$, and $\mu_t(dx)$ has a Radon–Nikodym derivative $\ell(x, t) = d\mu_t/dx$ with respect to Lebesgue measure dx on the real line. The local time $\ell(x, t)$ measures how much time $Y(s)$ spends at the point x during $0 < s < t$. Now the occupation density formula implies that $t = t(u) = \int_0^\infty \ell(x, u) dx$, which can be understood as adding up the time $Y(s)$ spends at all points $x > 0$. The local time has a scaling property $c^{1-1/\alpha} \ell(c^{-1/\alpha} x, c^{-1} t) = \ell(x, t)$ in distribution [31], and it follows that $t(ct) = ct(u)$ in distribution. Then $Z(ct) = c^{1/\alpha} Z(t)$, so that $Z(t)$ has the same scaling as $Y(t)$. It is known that the inverse local time is a nondecreasing Lévy process [7, p. 130]. However, it seems that the integral $t(u)$ is no longer Markovian. Hence, it seems difficult to prove that the probability distribution of $Z(t)$ is the same as $Y(t) \mid Y(t) > 0$.

Acknowledgements

The authors would like to thank Dr James F. Kelly, Naval Postgraduate School, who originally suggested that Zolotarev’s duality might be used to connect space- and time-fractional derivatives. Thanks also to Professor Yimin Xiao, Department of Statistics and Probability, Michigan State University, for helpful discussions.

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