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Abstract A continuous time random walk (CTRW) imposes a random waiting time between random particle jumps. CTRW limit densities solve a fractional Fokker-Planck equation, but since the CTRW limit is not Markovian, this is not sufficient to characterize the process. This paper applies continuum renewal theory to restore the Markov property on an expanded state space, and compute the joint CTRW limit density at multiple times.

Keywords Continuous time random walk · Fractional derivative · Anomalous diffusion · Renewal theory · Subordination · Time change · Levy process · Subdiffusion · Fractional dynamics

1 CTRW Limits

Random walk models are widely used for diffusive processes, to model the microscopic movements of random particles. Random walk limit densities solve a Fokker-Planck equation that provides a macroscopic model for diffusion. In the simplest case, J_k, $k = 1, 2, \ldots$ is a sequence of random jumps on $\mathbb{R}^d$, and each J_k is drawn from the same probability distribution with mean 0 and standard deviation 1. At each scale $\tau > 0$, the jumps J_k^τ are given by $\sqrt{\tau} J_k$, and the time between jumps is τ. Then the position of the random walker at time t and scale τ is

$$B^\tau(t) = \sum_{k=1}^{\lfloor t/\tau \rfloor} J_k^\tau, \tag{1}$$

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where $\lfloor x \rfloor$ denotes the largest integer not bigger than x. As τ decreases to 0, jumps become smaller and more frequent during the time interval $[0,t]$. In the limit $\tau \downarrow 0$, Donsker's theorem [1, Remark 4.17] implies that the distribution of paths $B^\tau(t)$ approaches a Brownian motion. An approximation of spatially inhomogeneous diffusions runs along the same lines, with a sequence of jumps J^τ_{k+1} whose means and standard deviations only depend on their current position $B^\tau(\tau k)$ and equal $\tau\mu(B^\tau(\tau k))$ resp. $\sqrt{\tau}\sigma(B^\tau(\tau k))$ for some functions $\mu(x)$ and $\sigma(x)$.

Continuous Time Random Walks (CTRWs) were introduced by Montroll and Weiss [2] as generalizations of Random Walks, in which the waiting times τ between jumps are replaced by positive random variables W_k. CTRWs are hence semi-Markov processes, as noted by Scher and Motroll [3]. The CTRW is now widely used to model subdiffusive processes in physics, hydrology, finance and biology [4–6]. We denote the scale dependence with W^τ_k, and for simplicity we assume that the waiting times W^τ_k, $k = 1, 2, \dots$ are drawn from the same distribution, which only depends on τ. The number of steps by time t is then no longer $\lfloor t/\tau \rfloor$ but given by the renewal process

$$N^\tau(t) = \max\left\{k:\ W^\tau_1 + \cdots + W^\tau_k \le t\right\}, \tag{2}$$

and the position of the random walker at time t is given by the CTRW

$$X^\tau(t) = \sum_{k=1}^{N^\tau(t)} J^\tau_k. \tag{3}$$

Two cases can occur: The mean of the waiting times at scale τ can be finite or infinite. If it is finite, then one scales the waiting times according to $W^\tau_k = \tau W_k$, and according to the law of large numbers $\tau N^\tau(t) \sim t/m$ for large t, where $m = \langle W_k \rangle$ denotes the mean of W_k. The process $X^\tau(t)$ will then converge pathwise to a limiting Brownian motion $B(t/m)$. Technically speaking, this is weak convergence of the associated probability measures on the space of right-continuous functions with left-hand limits in the Skorokhod J_1-topology [7]. If the waiting times W^τ_k have infinite mean, then the temporal scaling is different. Distributions with diverging mean are most easily classified by their heavy-tail parameter $\alpha \in (0,1)$ [1, Chapter 4]. Assume for instance that the waiting times are Pareto distributed such that the tail function satisfies

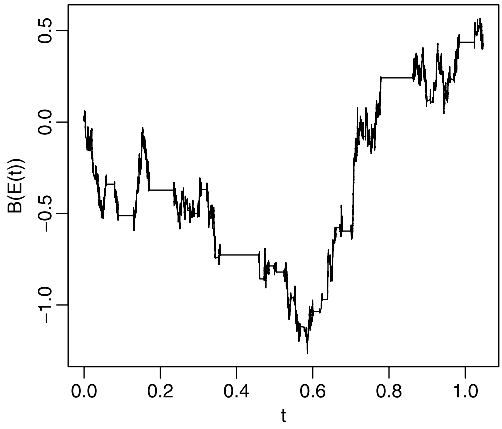
$$\mathbf{P}(W_k > t) \sim (1+t)^{-\alpha}/\Gamma(1-\alpha) \tag{4}$$

for large t, where $\Gamma(x)$ denotes the Gamma function. We then scale the waiting times via $W^\tau_k = \tau^{1/\alpha} W_k$, and similarly to the sum of jumps, we define the cumulative sum of waiting times as

$$Z^\tau(t) = \sum_{k=1}^{\lfloor t/\tau \rfloor} W^\tau_k. \tag{5}$$

This process can be viewed as a random walk in time with only positive jumps. In probability theory, the jump times $Z^\tau(\tau n)$ are called the "epochs" of the associated renewal process [8]. A generalized version of Donsker's theorem [9] shows that $Z^\tau(t)$ converges as $\tau \downarrow 0$ to a positively skewed α-stable Lévy process $Z(t)$ whose probability density has Laplace transform $\exp(-ts^\alpha)$ [1, Theorem 3.41]. This process has stationary independent increments, and $Z(t)$ has the same distribution as $t^{1/\alpha}Z(1)$. $Z(t)$ is a pure jump process with infinitely many jumps on finite intervals, and jumps of size $> z$ will occur at a Poisson rate with parameter $\bar{\nu}(z) = z^{-\alpha}/\Gamma(1-\alpha)$. We introduce the process *inverse to* $Z^\tau(t)$ via

Fig. 1 A typical particle trace $B(E(t))$ for Brownian motion time changed by an inverse 0.8-stable subordinator



$$E^\tau(t) = \inf\{s \geq 0\colon\ Z^\tau(s) > t\}. \tag{6}$$

Then one verifies that $E^\tau(t) = \tau(N^\tau(t) + 1)$, and hence the CTRW at scale τ can be written as

$$X^\tau(t) = B^\tau\big(E^\tau(t) - \tau\big). \tag{7}$$

In the scaling limit $\tau \downarrow 0$, $E^\tau(t)$ converges to $E(t) = \inf\{u > 0\colon\ Z(u) > t\}$, the process inverse to $Z(t)$ [10, Theorem 3.2]. Moreover, the composition of paths also converges in the scaling limit, and the CTRWs $X^\tau(t)$ converge to the *CTRW limit process*

$$X(t) = B\big(E(t)\big) \tag{8}$$

[10, Theorem 4.2], see also [11]. Replacing clock time t in the parent process $B(t)$ by the operational time $E(t)$ accounts for particle resting times between movements. Since $E(t)$ grows at the rate t^α, this time change results in a sub-diffusion, where a plume of particles spreads more slowly than a traditional diffusion. Figure 1 shows a typical sample path.

2 Fractional Dynamics

CTRW limit densities solve a time-fractional governing equation that provides a macroscopic model for sub-diffusion processes. We write $h_t(x)$ for the probability density of the operational time $E(t)$, that is $\mathbf{P}[E(t) \in dx] = h_t(x)\,dx$, and similarly we write $q_t(x)$ for the probability density of the diffusion process $B(t)$. Then by conditioning on $E(t)$, it follows that the probability density of the CTRW limit process $X(t) = B(E(t))$ is

$$p_t(x) = \int_0^\infty q_s(x) h_t(s)\,ds. \tag{9}$$

The time change of $B(t)$ by $E(t)$ has an analogue in terms of governing differential equations: Assume that $q_t(x)$ satisfies the Fokker-Planck equation (FPE)

$$\partial_t q_t(x) = \nabla_x^2\big[a(x)q_t(x)\big] - \nabla_x\big[b(x)q_t(x)\big] + q_0(x)\delta(t), \tag{10}$$

with diffusivity $a(x)$, drift $b(x)$, and initial particle density $q_0(x)$. Then $p_t(x)$ solves the *fractional* Fokker-Planck equation (FFPE)

$$\partial_t^\alpha p_t(x) = \nabla_x^2\big[a(x)p_t(x)\big] - \nabla_x\big[b(x)p_t(x)\big] + p_0(x)\frac{t^{-\alpha}}{\Gamma(1-\alpha)}, \tag{11}$$

where ∂_t^α denotes the Riemann-Liouville derivative of order α and $p_0(x) = q_0(x)$ [12–14]. If the coefficients $a(x)$ and $b(x)$ depend on space x *and* time t, a different FFPE holds [15].

The (non-fractional) FPE (10) completely determines the evolution of the diffusion $B(t)$: Given any particle distribution $q_{t_1}(x)$ at time t_1, one can calculate the distribution $q_{t_2}(x)$ at time t_2, update the starting condition to $q_{t_2}(x)$, calculate $q_{t_3}(x)$, and so forth. This is a simple consequence of the Markov property. Since $E(t)$ lacks the Markov property, $X(t) = B(E(t))$ is also non-Markov, and hence this formalism breaks down for the FFPE. This problem has been discussed in the physics literature [16], where the joint governing equation of $X(t)$ at multiple times was recorded. In the next section, we show how to solve those equations, by computing the joint density of $X(t)$ at multiple times.

3 Continuum renewals

CTRW renewal theory is very general, allowing for space- and time-dependent jumps and waiting times, jump lengths that depend on the associated waiting time (the coupled case), and scale dependent CTRW as in [20]. To simplify the presentation, we restrict attention to the "operational time" $E(t)$ and "forward recurrence time" $R(t)$. See [17] for complete mathematical details.

3.1 The Discrete Setting

We now study the renewal property of CTRWs and their limit processes. CTRWs are also called Markov renewal processes, due to the following property: after each jump, the walker forgets the past, and the future trajectory only depends on the current position in space. Renewals occur at the random set of jump times

$$\mathbf{M}^\tau = \big\{Z^\tau(t)\colon\ t \geq 0\big\}. \tag{12}$$

The (random) time of the first renewal after a fixed time t is

$$H^\tau(t) = \inf\big\{\mathbf{M}^\tau \cap (t,\infty)\big\}, \tag{13}$$

that is, the first point in $\mathbf{M}^\tau$ to the right of t. By definition of $E^\tau(t)$,

$$H^\tau(t) = Z^\tau\big(E^\tau(t)\big). \tag{14}$$

The forward recurrence time or remaining lifetime is defined as $R^\tau(t) = H^\tau(t) - t$. The joint dynamics of $(X^\tau(t), R^\tau(t))$ now runs as follows: $X^\tau(t)$ remains fixed as $R^\tau(t)$ decreases to 0 with speed 1. When it reaches 0, $X^\tau(t)$ jumps and $R^\tau(t)$ is reset to take the value of the next waiting time. Since at every time t the future evolution depends solely on the current state $(X^\tau(t), R^\tau(t))$, the process is Markov. See Fig. 2 for an illustration.

3.2 The Scaling Limit

In the scaling limit $\tau \downarrow 0$, the discrete process $Z^\tau(t)$ converges to a strictly increasing α-stable Lévy process $Z(t)$. The random set $\mathbf{M}^\tau$ converges in distribution to the set $\mathbf{M} = \{Z(t)\colon\ t \geq 0\}$ constructed by deleting the intervals $[Z(t-), Z(t))$ from the positive real line. Since there are infinitely many jumps on finite time intervals, $\mathbf{M}$ has a Cantor-set like structure; in fact, $\mathbf{M}$ is a fractal of dimension α [18].

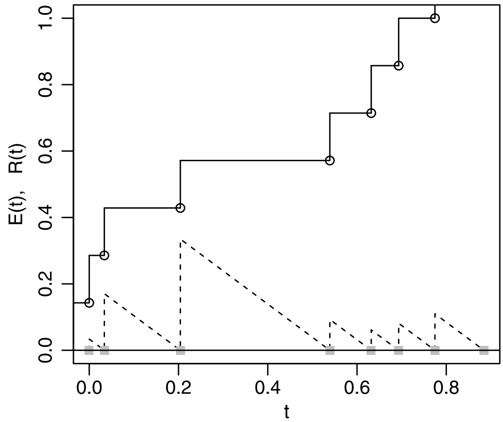


Fig. 2 Operational time ($E(t)$, *solid line*, discontinuous) and remaining lifetime ($R(t)$, *dashed line*) vs. physical time t at the scale $\tau = 1/7$. The regenerative set **M** is shaded in grey on the t-axis

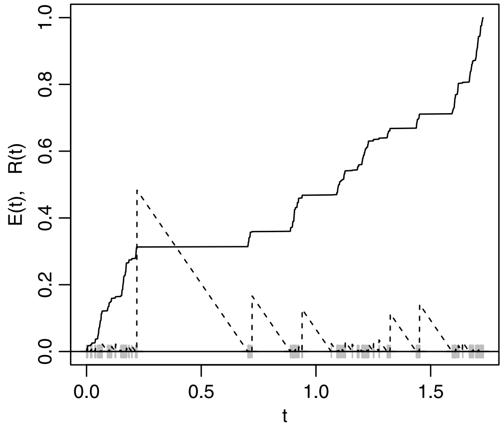


Fig. 3 The same quantities as in Fig. 2, at the scaling limit $\tau = 0$. $E(t)$ is now continuous. The underlying subordinator $Z(t)$ is 0.7-stable, and the regenerative set (*grey*) is a fractal of dimension 0.7

The forward recurrence time is $H(t) = Z(E(t))$, and the remaining lifetime $R(t) = H(t) - t$ counts down the time until the next renewal (see Fig. 3). When $R(t)$ reaches 0, the CTRW limit process $X(t)$ is renewed, and behaves as if started from the current position in space at time 0. Since the parent process $B(t)$ is a continuous diffusion, the limit process $X(t)$ does not jump at a renewal. The Markov property of the joint process $(X(t), R(t))$ still holds in the limit.

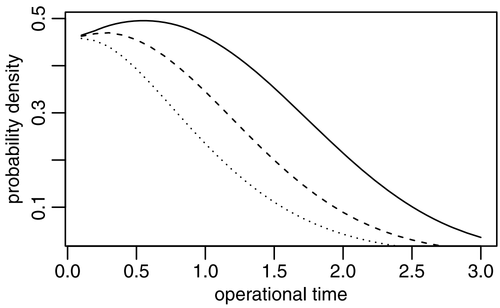
4 The Joint Density of Operational and Recurrence Time

In this section we calculate the joint distribution of $E^\tau(t)$ and $R^\tau(t)$. We consider the event that $E^\tau(t) \le x$ and simultaneously $R^\tau(t) > r$ for arbitrary positive numbers x and r. We first introduce the measure on $[0, \infty) \times [0, \infty)$ defined for arbitrary closed sets $I, J \subset [0, \infty)$ by

$$U^\tau(I \times J) = \left\langle \tau \sum_{k=1}^{\infty} \delta_{\tau k}(I) \delta_{Z^\tau(\tau k)}(J) \right\rangle, \qquad (15)$$

where δ_x denotes the Dirac measure concentrated at x, and where $\langle \cdot \rangle$ denotes expectation or the ensemble average taken over all paths of $Z^\tau(t)$. It measures τ times the mean amount of

Fig. 4 Sections $x \mapsto h_t(x,r)$ of the joint probability density function (21) with index $\alpha = 0.6$ for operational time $x = E(t)$ and remaining lifetime $r = R(t)$ at clock time $t = 1$ for $r = 0$ (*solid*), 0.1 (*dashed*), and 0.5 (*dotted*)



values k such that τk lies in the set I and simultaneously $Z^\tau_{\tau k}$ lies in the set J. If $I = \{\tau k\}$, then $U^\tau(I \times J)/\tau$ is the probability that $Z^\tau_{\tau k}$ lies in J. We now observe that the event $E^\tau(t) = \tau k$, $R^\tau_t > r$ can be written as

$$Z^\tau\big(\tau(k-1)\big) \le t, \qquad Z^\tau(\tau k) > t + r, \tag{16}$$

and that this is equivalent to

$$Z^\tau\big(\tau(k-1)\big) \le t, \qquad W^\tau_k > t + r - Z^\tau\big(\tau(k-1)\big). \tag{17}$$

The probability of the latter event can now be written as

$$\int_0^t \int_{\{\tau k\}} \frac{U^\tau(y,s)}{\tau} \bar{\nu}^\tau(t+r-s)\, dy\, ds, \tag{18}$$

where $\bar{\nu}^\tau(t)$ denotes the tail probability $\mathbf{P}(W^\tau_k > t)$. Integrating over $y \in [0,x]$ instead of $y = \tau k$ we have the probability of the event $E^\tau \le x$, $R^\tau_t > r$. If we now let the scale parameter $\tau \downarrow 0$, we find

$$\tau^{-1}\bar{\nu}^\tau(t) \to t^{-\alpha}/\Gamma(1-\alpha) = \bar{\nu}(t). \tag{19}$$

Moreover, the measures U^τ converge to a continuous measure U whose density is $u(x,s)$, and where for fixed $x > 0$ the function $s \mapsto u(x,s)$ is the probability density of $Z(x)$. Hence the probability of the event $E(t) \le x$, $R(t) > r$ is

$$\int_0^t \int_0^x u(y,s)\bar{\nu}(t+r-s)\, dy\, ds, \tag{20}$$

and we have derived the joint density $\mathbf{P}(E(t) \in dx, R(t) \in dr) = h_t(x,r)\, dx\, dr$ of the limiting operational time and remaining lifetime:

$$h_t(x,r) = \int_0^t u(x,s)\nu(t+r-s)\, ds, \tag{21}$$

valid for positive x and r, and where $\nu(z) = -\partial_z \bar{\nu}(z)$ is the density of the jump measure of $Z(t)$. The probability density of $E(t)$ computed in [20, (3.11)] can be recovered by integrating (21) over $r > 0$. The symbol h should not be confused with the probability density function of the first waiting time in an aging CTRW, as introduced in [19].

Figure 4 shows sections $x \mapsto h_t(x,r)$ of the joint probability density function (21) for several different values of the remaining lifetime r. The computation used the `dstable` command in the R package `fbasics` to compute the stable density $u(x,s)$ in (21). The R code that produce this graph is available from the authors upon request.

Equation (21) applies to any CTRW limit, assuming that $(B(t), Z(t))$ is a Markov process, with $Z(t)$ strictly increasing [17]. For example, if $Z(t)$ is *tempered* α-stable [21–23], it holds with a tempered stable density $s \mapsto u(x,s)$ of index $0<\alpha<1$ and jump intensity $\nu(t) = \alpha t^{-\alpha-1}\exp(-\lambda t)/\Gamma(1-\alpha)$, where $\lambda > 0$ is a tempering parameter. For coupled Continuous Time Random Walks, the argument extends, using a space-time jump intensity $\nu(x,t)$ to model simultaneous increments of $B(t)$ and $Z(t)$, see [17]. It is not straightforward to apply our formalism to a CTRW with correlated waiting times [24–26], since $Z(t)$ is not Markovian in that case.

5 Probability Densities at Multiple Times

Using the joint density $h_t(x,r)$ of operational and recurrence time in (21), we can calculate the distribution of the operational time $E(t_k)$ at two or more consecutive times. Laplace transforms of the joint distributions of $E(t_k)$ at two times were calculated in [27, 28], and double-fractional differential equations were derived in [16]. When $B(t)$ is a Poisson process, joint distributions of the fractional Poisson process $B(E_t)$ were calculated in [29].

With the theory set up as described, we calculate the distribution of the operational time at two consecutive times t_1, t_2 as follows: Given that the operational time $E(t)$ equals x at the physical time $t=0$ and given that there will be an initial lag $R(0)=\ell \geq 0$ until the next progression of the operational time, we let $h_t(x,\ell;y,r)$ be the probability density of $E(t)=y$ and $R(t)=r$. This density then equals

$$h_t(x,\ell;y,r) = \begin{cases} h_{t-\ell}(y-x,r), & t>\ell \\ \delta(y-x)\delta(r-(\ell-t)), & t\leq \ell. \end{cases} \tag{22}$$

For $0\leq t_1 \leq t_2$, the joint density of $E(t_1)=x_1$ and $E(t_2)=x_2$ then equals

$$h_{t_1,t_2}(x_1,x_2) = \int_0^\infty h_{t_1}(0,0;x_1,r_1)\int_0^\infty h_{t_2-t_1}(x_1,r_1;x_2,r_2)\,dr_2\,dr_1, \tag{23}$$

and similar formulas hold for an arbitrary number of times t_k. Now suppose that $q_t(x,y)$ is the transition probability density of the time-homogeneous Markov process $y=B(t+s)$ given $x=B(s)$. Then the Chapman-Kolmogorov equation implies that $q(x,y,s,t) = q_{t-s}(x,y)q_s(x_0,x)$ is the joint probability density of $(x,y)=(B(s),B(t))$ given initial particle location $B(0)=x_0$, and so the joint density of the fractional diffusion process $X(t)=B(E(t))$ at times t_1,t_2 is

$$p_{t_1,t_2}(x,y) = \int_0^\infty \int_0^\infty q(x,y,u,v)h_{t_1,t_2}(u,v)\,dv\,du. \tag{24}$$

In a similar manner, one can calculate the joint probability density of the fractional diffusion process $X(t)=B(E(t))$ at times $t_1,\dots,t_n$.

For any time $s>0$, the particle displacement $X(t+s)-X(s)$ is conditionally independent of $X(t)$ given the remaining lifetime $R(s)$. If $R(s)\geq t$, then the particle remains at rest, and $X(t+s)-X(s)=0$. Otherwise, if $0\leq R(s)<t$, then the distribution of $X(t+s)-X(s)$ given $R(s)=r$ is the same as that of $X(t-r)$, since $X(t)$ has a renewal point at time $s+r$. Figure 5 illustrates the effect of the remaining lifetime on particle displacement, showing the distribution of the displacement $X(t+s)-X(s)$ for different values of $r=R(s)<t$, in the case where $X(t)$ is governed by the fractional Fokker-Planck equation (11) with $a(x)\equiv 1$ and $b(x)\equiv 0$. These curves are similar in shape to a normal density, but with a sharper peak, and heavier tails. Note that, for example, the curve for $t=3$ and $R(s)=2.9$ is identical to the probability density function (9) with $t=0.1$, and was computed using the R code in [1, Example 5.13].

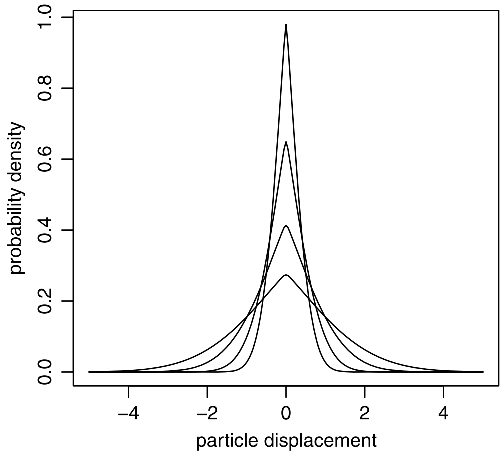


Fig. 5 Conditional probability density function of particle displacement $X(t+s)-X(s)$ for $t=3$ given remaining lifetime $R(s)=0$ (*widest curve*), 2, 2.7, and 2.9 (*narrowest curve*). Here $X(t)$ has governing equation (11) with $a(x)\equiv 1$ and $b(x)\equiv 0$

6 Joint Governing Equation

In this section, we derive the governing equation of the probability density $h_t(x,r)$ in (21). Pseudo-differential operators on $\mathbb{R}^n$ are of the form $\psi(i\nabla_x)$, where for our purposes $-\psi(k)$ is a negative definite function on $\mathbb{R}^n$ and

$$\psi(i\nabla_x)f(x)=(2\pi)^{-n}\int e^{-ik\cdot x}\psi(k)\hat{f}(k)\,dk, \tag{25}$$

where $\hat{f}(k)=\int e^{ik\cdot x}f(x)\,dx$ denotes the Fourier transform of a function f. An instructive example is the negative Laplacian $-\nabla_x^2$, whose action corresponds to a multiplication with $\psi(k)=\|k\|^2$ in Fourier-space. Jurlewicz et al. [30] have shown that if $(B(t),Z(t))$ is a Lévy process in $\mathbb{R}^d\times\mathbb{R}^+$ (e.g. if $B(t)$ is Brownian motion and $Z(t)$ an α-stable increasing Lévy process) whose double Fourier-transform is

$$\exp\bigl(-t\psi(k,s)\bigr)=\bigl\langle\exp\bigl(ik\cdot B(t)+isZ(t)\bigr)\bigr\rangle, \tag{26}$$

then the probability density $\rho_t(x)$ of $X(t)=B(E(t))$ satisfies

$$\psi(i\nabla_x,i\partial_t)\rho_t(x)=\delta(x)\int_t^\infty\phi(z)\,dz. \tag{27}$$

Here $E(t)$ is again inverse to $Z(t)$, and $\phi(z)$ denotes the density of the jump measure of $Z(t)$. For example, if $B(t)$ is Brownian motion with covariance matrix $2tI$ and $Z(t)$ is an independent α-stable subordinator, then $\psi(i\nabla_x,i\partial_t)=\partial_t^\alpha-\nabla_x^2$ and (27) reduces to the fractional Fokker-Planck equation (11) with $a\equiv 1$ and $b\equiv 0$.

Now write $(E(t),H(t))=B(E(t))$, where $B(t):=(t,Z(t))$, and note that the Lévy process $(B(t),Z(t))$ has Fourier symbol

$$\psi(k_1,k_2,s)=-ik_1+\bigl(-i(k_2+s)\bigr)^\alpha. \tag{28}$$

The joint probability density $\rho_t(x,y)$ of $E(t)=x$ and $H(t)=y$ hence satisfies the pseudo-differential equation (27), and since $R(t)+t=H(t)$, it follows that $h_t(x,y+t)=\rho_t(x,y)$ solves the same equation:

$$\bigl[\partial_x+(\partial_t+\partial_y)^\alpha\bigr]h_t(x,y+t)=\delta(x)\delta(y)\frac{t^{-\alpha}}{\Gamma(1-\alpha)}. \tag{29}$$

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