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Governing equations and solutions of anomalous random walk limits

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Continuous time random walks model anomalous diffusion. Coupling allows the magnitude of particle jumps to depend on the waiting time between jumps. Governing equations for the long-time scaling limits of these models are found to have fractional powers of coupled space and time differential operators. Explicit solutions and scaling properties are presented for these equations, which can be used to model flow in porous media and other physical systems.

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I. INTRODUCTION

The scaling limit of a random walk often generates a governing equation that is extremely useful, since it can be solved in a variety of boundary and initial value problems. The simplest random walk converges to the familiar Brownian motion with a second-order diffusion equation governing the probabilistic particle location. However, when some of the moments of the jump size and/or waiting time diverge, a Brownian motion is never reached. The diffusion is called anomalous in this case, since the growth of the diffusion may be slower or faster than predicted by Brownian motion. The continuous time random walk (CTRW) method [1,2] allows determination of the limiting processes when the particle jumps have infinite variance [3–7] and/or the waiting times between particle jumps have infinite mean [3,4,7–10]. When the jump sizes and waiting times are independent, the governing equation contains fractional-order space and/or time derivatives [5,8,11–15]. The limit process may be superdiffusive or subdiffusive. In this paper we specify the technique for determining the limit process and the governing equation for random walks, where the jump sizes and waiting times are linked or coupled. We show that the governing equation contains fractional powers of grouped space and time derivative operators and we compute the Green's function solutions where possible.

In the coupled case, the waiting time between jumps affects the size of the subsequent jump [2,16]. These coupled CTRW have been reported in a variety of physical systems [8,17]. In hydrodynamics, the coupled motions have been used to describe transport in chaotic [18,19] and turbulent [20] flows, and flow confined to percolation networks [21]. Long waiting times may be preferentially followed by small jumps for dissolved pollutants moving through aquifer material, since clay particles tend to lower the velocity of mobile water, and also have large surface charges that strongly sorb charged or polar solutes for random amounts of time. A correlation between velocity and sorption strength is either measured or assumed for many pollutants, including organic solvents and radionuclides [22].

Space-time coupling blends subdiffusive and superdiffusive effects, resulting in a different kind of limiting process governed by a model equation involving coupled space-time fractional derivatives. These equations are useful to model flow in porous media and other physical systems characterized by a link or coupling between the subdiffusive tendencies caused by particle sticking or trapping, and the superdiffusive influence of very large particle jumps.

II. THE MASTER LIMIT EQUATION

Scaling limits and governing equations for CTRW can be computed via the Montroll-Weiss *master equation* [1,2,16]. A random waiting time J is followed by a particle jump of random size Y, defining the random *transition* vector (Y,J). Additional transitions are independent and identically distributed, but each Y and J may depend on each other. The master equation

$$P(k,s)=\frac{1-g(s)}{s}\frac{1}{1-p(k,s)} \tag{1}$$

gives the Fourier-Laplace transform $(x\mapsto k,\ t\mapsto s)$ of particle density $P(x,t)$ in terms of the joint probability density $p(x,t)$ of (Y,J) and the marginal density $g(t)=\int p(x,t)dx$ of the waiting time J. A simple uncoupled CTRW with finite mean waiting time and finite variance particle jumps has $g(s)=1-s+o(s)$ and $p(k,s)=[1-s+o(s)][1-k^2+o(k^2)]$ for small s,k. Rescale in time and space by replacing s by cs and k by $c^{1/2}k$, and substitute into Eq. (1). Then, as $c\to 0$ the higher order terms vanish and

$$P(c^{1/2}k,cs)\to Q(k,s)=\frac{1}{s+k^2}.$$

Inverting the Fourier-Laplace transform of the limit yields $Q(x,t)=(4\pi t)^{-1/2}e^{-x^2/4t}$, so the scaling limit of this CTRW is a classical Brownian motion. The limit satisfies (s

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$+k^2)Q(k,s)=1$ and inverting yields the governing equation $(\partial/\partial t-\partial^2/\partial x^2)Q(x,t)=\delta(x)\delta(t)$ for this diffusion. A useful short-cut is to approximate $g(s)\approx 1-s$ and $p(k,s)\approx 1-s-k^2$ and ignore product terms in Eq. (1), but one must bear in mind the proper rescaling in time and space that makes these terms vanish. Infinite mean waiting times $(0<\beta<1)$ and symmetric infinite variance jumps $(0<\alpha<2)$ lead to $g(s)=1-s^\beta+o(s^\beta)$ and $p(k,s)=[1-s^\beta+o(s^\beta)][1-|k|^\alpha+o(|k|^\alpha)]$, and the proper rescaling $s=c^{1/\beta}s$ and $k=c^{1/\alpha}k$ leads to a scaling limit $Q(k,s)=s^{\beta-1}/(s^\beta+|k|^\alpha)$, whose stochastic equivalent and fractional-order governing equation are discussed in Refs. [7,13–15]. This procedure, based on the master equation, works well for uncoupled CTRWs because the density $p(x,t)$ is a product of the independent space and time marginals.

Coupled CTRWs present a more difficult challenge, since the density $p(x,t)$ does not decompose into a product of the marginals, making the appropriate rescaling more subtle. The mathematical analysis in Ref. [23] resolves this difficulty using operator stable limit theory [24–26] for the joint (possibly dependent) space-time random vector (Y,J). The resulting *master limit equation*

$$Q(k,s)=\frac{s^{\beta-1}}{\psi(k,s)} \tag{2}$$

gives the scaling limit of any coupled CTRW with infinite mean waiting time $(0<\beta<1)$. Inverting Eq. (2) leads to the governing equation

$$\psi\left(i\frac{\partial}{\partial x},\frac{\partial}{\partial t}\right)Q(x,t)=\delta(x)\frac{t^{-\beta}}{\Gamma(1-\beta)} \tag{3}$$

involving a coupled space-time fractional derivative operator. The Lévy representation [26] gives the Fourier-Laplace symbol of this operator as

$$\psi(k,s)=\int_0^\infty\int_{-\infty}^\infty(1-e^{-st}e^{ikx})\ell(x,t)dx\,dt \tag{4}$$

in terms of the Lévy density $\ell(x,t)$ (also called the jump intensity [27,28]) of the space-time limit process. Assuming that (Y,J) obeys a general limit theorem, the Lévy density decomposes into

$$\ell(x,t)=t^{-m}f(t^{-m}x)\phi_1(t), \tag{5}$$

where $f(x)$ can be any probability density, $\phi_1(t)=K\beta t^{-\beta-1}$ is the Lévy density of the β-stable subordinator (K is a constant), and $m>\beta/2$ is the coupling parameter that links the jump size and waiting time. Formula (4) is valid when $m>\beta$, $f(x)$ is symmetric, or $\int xf(x)dx=0$. An extended form of Eq. (4) applies in other cases [23] and is not listed here for brevity. For an uncoupled CTRW, a different form (10) of the Lévy density applies (shown in a later section).

Many different coupled CTRW models converge to the same limit, and every possible limit can be obtained using a simple CTRW, where J has a stable density with Laplace transform $g(s)=e^{-s^\beta}$ and the conditional density of Y given $J=t$ is $t^{-m}f(t^{-m}x)$, so that $f(x)$ is the *conditional* distribution of Y given $J=1$. A heuristic link with the master equation (1) can be obtained using $g(s)\approx 1-s^\beta$ and $p(k,s)\approx 1-\psi(k,s)$ for small s,k in the appropriate space-time rescaling. The Fourier-Laplace symbol $\psi(k,s)$ has a scaling property $c\psi(k,s)=\psi(c^{1/\alpha}k,c^{1/\beta}s)$, where $\alpha=\beta/m$ is the tail parameter of the *unconditional* distribution of the jump size Y. Then Eq. (2) leads to $Q(k,ct)=Q(c^m k,t)$, where $m=\beta/\alpha$, so this coupled CTRW model is subdiffusive for $m<1/2$, diffusive for $m=1/2$, and superdiffusive in the remaining case $m>1/2$. We give some example immediately.

III. COUPLED GOVERNING EQUATIONS AND SOLUTIONS

Shlesinger *et al.* [3] consider a coupled CTRW model, where particle jump size Y is normal mean zero with variance $2t$ when the waiting time $J=t$. The master limit equation reveals the governing equation for the CTRW limit and its explicit solution. Since the space-time limit of (Y,J) only depends on the tail behavior, any CTRW with a similar behavior will lead to the same limit. The conditional density of Y given $J=t$ is $(4\pi t)^{-1/2}e^{-x^2/4t}=t^{-m}f(t^{-m}x)$ with $f(x)=(4\pi)^{-1/2}e^{-x^2/4}$ and $m=1/2$. Using this form in Eq. (5), along with $\int_0^\infty(1-e^{-st})\phi_1(t)dt=s^\beta$ and $\mathcal{F}[f(x)]=e^{-k^2}$, the Lévy representation (4) gives $\psi(k,s)=(s+k^2)^\beta$ in the simplest case $K\Gamma(1-\beta)=1$. Here, $\alpha=2\beta$ and the unconditional distribution of Y is symmetric α stable. The coupling produces a finite variance limit even though the individual jumps have infinite variance. Formula (3) gives the coupled governing equation

$$\left(\frac{\partial}{\partial t}-\frac{\partial^2}{\partial x^2}\right)^\beta Q(x,t)=\delta(x)\frac{t^{-\beta}}{\Gamma(1-\beta)}.$$

Inverting Eq. (2) using $\mathcal{L}[t^{q-1}]=s^{-q}/\Gamma(q)$ gives

$$Q(x,t)=\int_0^t(4\pi u)^{-1/2}e^{-x^2/4u}t^{-1}b(t^{-1}u)du, \tag{6}$$

where $b(u)=u^{\beta-1}(1-u)^{-\beta}/\Gamma(\beta)\Gamma(1-\beta)$ is a beta density. The integral (6) is a mixture of Gaussian densities whose random variance is governed by a β density. This model is diffusive since $m=1/2$, but the plume has a sharp non-Gaussian peak at $x=0$ (Fig. 1) due to the infinite mean $(\beta<1)$ waiting times. As $\beta\uparrow 1$ the particle location density converges to the limiting $(\beta=1)$ Gaussian case (Fig. 2).

Shlesinger *et al.* [3] also consider a more general coupled CTRW model with $f(x)=(4\pi)^{-1/2}e^{-x^2/4}$ and an arbitrary coupling parameter $m>\beta/2$. Then $\alpha=\beta/m<2$, and the jump size Y is tail equivalent to an α-stable random variable. In this case, similar calculations [23] give

$$\psi(k,s)=\int_0^\infty(1-e^{-st}e^{-k^2t^{2m}})\phi_1(t)dt, \tag{7}$$

which cannot be written in closed form, but it is easy to verify directly that $Q(x,ct)=c^{-m}Q(c^{-m}x,t)$, showing that this CTRW is subdiffusive for $m<1/2$, diffusive in the original case $m=1/2$, and superdiffusive when $m>1/2$ [23].

RAPID COMMUNICATIONS

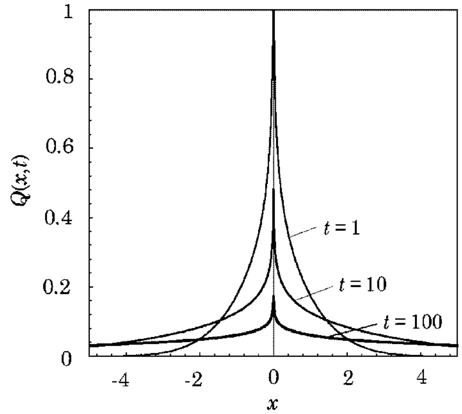

FIG. 1. Particle densities $Q(x,t)$ in the coupled CTRW model (6) with $\beta=1/2$ have sharp peaks at $x=0$ due to infinite mean waiting times.

Here, the master limit equation provides analytical verification of asymptotic results in Ref. [3].

Another CTRW [29–31] considers a tight coupling with $|Y|=J$, so that $f(x)=[\delta(x-1)+\delta(x+1)]/2$, $m=1$, and the tail parameter of Y is $\alpha=\beta$. The variable $|Y|$ is α stable but Y is not. Here, the Lévy density (5) is $\ell(x,t)=(1/2)[\delta(x-t)+\delta(x+t)]\phi_1(t)$, the Fourier-Laplace symbol (4) reduces to $\psi(k,s)=[(s-ik)^\beta+(s+ik)^\beta]/2$, and Eq. (3) gives

$$\left[\left(\frac{\partial}{\partial t}+\frac{\partial}{\partial x}\right)^\beta+\left(\frac{\partial}{\partial t}-\frac{\partial}{\partial x}\right)^\beta\right]Q(x,t)=\frac{2\,\delta(x)t^{-\beta}}{\Gamma(1-\beta)}.$$

Since $m=1$ this ballistic CTRW scales linearly with time [31]. Recently, Barkai [32] computed $Q(k,s)$ for this model by completely different methods. That paper also develops exact preasymptotic CTRW solutions, investigates rates of convergence to the long-time limit, and discusses the problem of obtaining governing equations in the case $1<\beta<2$.

A wide variety of coupled governing equations can be obtained and solved in a similar manner. If the coupling parameter $m=1/\gamma$, then $\alpha=\gamma\beta$, the Lévy density $\ell(x,t)=t^{-1/\gamma}f(t^{-1/\gamma}x)\phi_1(t)$, and Eq. (4) leads to

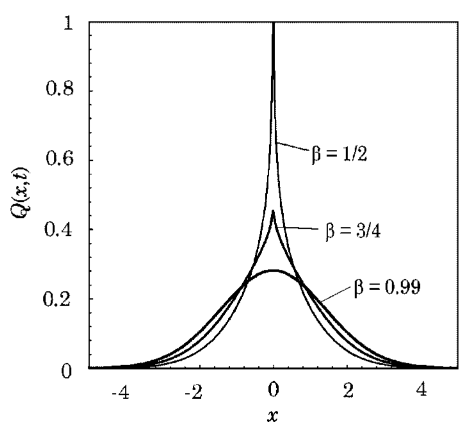

FIG. 2. Particle densities $Q(x,t)$ in the coupled CTRW model (6) (shown here at $t=1$) converge to a Gaussian as $\beta\uparrow 1$.

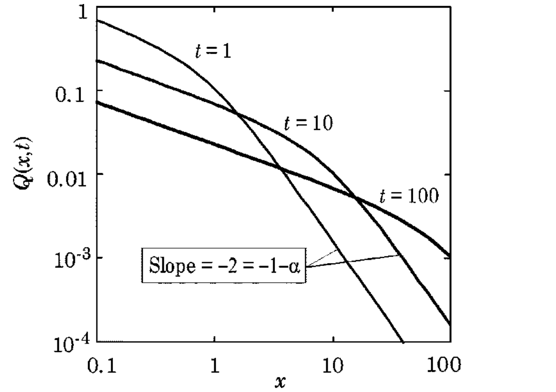

FIG. 3. Particle densities $Q(x,t)$ for a coupled CTRW with $f(x)$ standard Cauchy and $\beta=1/2$ in Eq. (9) retain the Cauchy power law tails.

$$\psi(k,s)=\int_0^\infty[1-e^{-st}f(t^{1/\gamma}k)]\phi_1(t)dt. \tag{8}$$

If $f(x)$ is a γ-stable density then $f(k)=e^{-\psi_2(k)}$ with $\psi_2(k)=Cp(-ik)^\gamma+C(1-p)(ik)^\gamma$ so $f(t^{1/\gamma}k)=e^{-t\psi_2(k)}$. Here, C is a positive constant and $0\leqslant p\leqslant 1$ is the weight on forward versus backward jumps (i.e., the skewness). Then $\psi(k,s)=[s+\psi_2(k)]^\beta$ and the governing equation for $\gamma\neq 1$ is

$$\left(\frac{\partial}{\partial t}-p\frac{\partial^\gamma}{\partial x^\gamma}-(1-p)\frac{\partial^\gamma}{\partial(-x)^\gamma}\right)^\beta Q(x,t)=\frac{\delta(x)t^{-\beta}}{\Gamma(1-\beta)},$$

in the simplest case $C\Gamma(1-\gamma)=1$. Inverting Eq. (2) gives

$$Q(x,t)=\int_0^t u^{-1/\gamma}f(u^{-1/\gamma}x)t^{-1}b(t^{-1}u)du, \tag{9}$$

where $b(u)=u^{\beta-1}(1-u)^{-\beta}/\Gamma(\beta)\Gamma(1-\beta)$ is a beta density. Equation (9) reduces to the form (6), when $\gamma=2$ and $f(x)=(4\pi)^{-1/2}e^{-x^2/4}$. When $\gamma=1$ and $f(x)=\pi^{-1}(1+x^2)^{-1}$ (a standard Cauchy), formula (8) evaluates to $\psi(k,s)=(s+|k|)^\beta$ and then Eq. (9) solves

$$\left(\frac{\partial}{\partial t}+\sqrt{-\frac{\partial^2}{\partial x^2}}\right)^\beta Q(x,t)=\delta(x)\frac{t^{-\beta}}{\Gamma(1-\beta)},$$

using $|k|=\sqrt{-(-ik)^2}$. The overall shape is similar to Fig. 1 but in this case the diffusing particle density has power law tails (Fig. 3).

IV. THE UNCOUPLED CASE

For uncoupled CTRW limits the coupled form of the Lévy density (5) is replaced by

$$\ell(x,t)=\delta(x)\phi_1(t)+\delta(t)\phi_2(x), \tag{10}$$

since for independent components the Lévy density must be concentrated on the coordinate axes [23,33]. Here, the spatial component $\phi_2(x)=Cp\alpha x^{-\alpha-1}H(x)+C(1-p)\alpha|x|^{-\alpha-1}H(-x)$ is the Lévy density of an α-stable random variable [23], and $H(x)$ is the Heaviside indicator function. Now Eq. (4) gives $\psi(k,s)=s^\beta-(-ik)^\alpha$ for the completely skewed case $p=1$, using the constants $K\Gamma(1-\beta)=1$ and $C\Gamma(1-\alpha)=1$. Then Eq. (3) becomes

$$\left(\frac{\partial^\beta}{\partial t^\beta}-\frac{\partial^\alpha}{\partial x^\alpha}\right)Q(x,t)=\delta(x)\frac{t^{-\beta}}{\Gamma(1-\beta)},$$

which is equivalent to the fractional kinetic equation of Zaslavsky [7,13]. The explicit solution

$$Q(x,t)=\frac{t}{\beta}\int_0^\infty q(x,t)g(tu^{-1/\beta})u^{-1/\beta-1}du \qquad (11)$$

to this fractional Cauchy problem [34] is the inverse Lévy transform [14] of the Green's function solution $q(x,t)$ to the Cauchy problem $\partial q(x,t)/\partial t=Lq(x,t)$ [13,15], where the spatial derivative operator $L=p\partial^\alpha/\partial x^\alpha+(1-p)\partial^\alpha/\partial(-x)^\alpha$, when $C\Gamma(1-\alpha)=1$. Scaling properties for uncoupled CTRW limits and extensions to vector jumps are discussed in [9,15]. The integral (11) is a scaled mixture of stable densities governed by a Mittag-Leffler density, in contrast to the beta density that governs the scale mixtures (6) and (9) for coupled CTRW limits.

V. SUMMARY

Coupled CTRWs link the waiting time between particle jumps with the ensuing jump size. Operator stable central limit theory for coupled space-time jump vectors leads to a master limit equation (2) for the Fourier-Laplace transform of CTRW scaling limit densities. Inverting reveals governing equations that employ coupled space-time fractional derivative operators. Explicit analytical solutions and scaling properties are available for many cases of interest. Coupled space-time equations are useful models for flow in porous media and other physical systems, where the delay between particle jumps affects the subsequent jump magnitude.

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