

## Anomalous diffusion, stable processes, and generalized functions

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The evolution equations in real space and time corresponding to a class of anomalous diffusion processes are examined. As special cases, evolution equations corresponding to stable processes are derived using the theory of generalized functions, recovering some known results differently interpreted, and an evolution law for stable processes of order unity.

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There has been a recent preoccupation in physics with the problem of “anomalous diffusion” [1,2], although stochastic transport processes that are other than classical diffusion have been of interest for many years [3–7]. Consider a random process that governs the position  $\mathbf{R}(t)$  of a moving particle at time  $t$ , and let the average or expectation be denoted by angular brackets. The variance of the position

$$\text{Var}\{\mathbf{R}(t)\} = \langle |\mathbf{R}(t) - \langle \mathbf{R}(t) \rangle|^2 \rangle = \langle |\mathbf{R}(t)|^2 \rangle - |\langle \mathbf{R}(t) \rangle|^2,$$

measures the spread of the process. For an initially localized ensemble of noninteracting particles,  $\sqrt{\text{Var}\{\mathbf{R}(t)\}}$  is a measure of the diameter of the “plume” produced as the system evolves.

Suppose that the variance for the process with initial condition  $\mathbf{R}(0) = \mathbf{0}$  evolves as

$$\text{Var}\{\mathbf{R}(t)\} \sim L(t)t^{2\nu} \quad \text{as } t \rightarrow \infty,$$

where  $L(t)$  is slowly varying in the sense that for each fixed  $\lambda > 0$ ,  $\lim_{t \rightarrow \infty} L(\lambda t)/L(t) = 1$ . Then there is a well-defined exponent  $\nu$  governing the process, and roughly speaking,  $\mathbf{R}(t) \approx t^\nu$ . The stochastic transport process is called *normal diffusion* if  $\nu = 1/2$ , and *anomalous diffusion* otherwise. Anomalous diffusion is classified as *subdiffusion* if  $0 < \nu < 1/2$  and *superdiffusion* if  $\nu > 1/2$ . The superdiffusive case is sometimes further divided, with  $\nu \geq 1$  called *ballistic*, and may be augmented with those processes for which  $\text{Var}\{\mathbf{R}(t)\} = \infty$  for all  $t > 0$ , which in some sense corresponds to  $\nu = \infty$ .

Models based on the Wiener process, limits of random walks in discrete time with finite mean-square displacement per step, and limits of continuous-time random walks with finite mean time between steps all produce normal diffusion if the process lives in Euclidean space. Subdiffusion may occur when a continuous-time random walk has infinite mean time between steps, and is also found in some quenched random environment problems [8,9]. Extreme superdiffusion [ $\text{Var}\{\mathbf{R}(t)\} = \infty$ ] follows when the individual constituent displacements have infinite variance [4,7]. It is harder to produce less drastic superdiffusion, or to derive models that encompass all possible qualitative behaviors as a few parameters are tuned.

Continuous-time random walk models, with the time between steps and the length of a step correlated [5–7,10], represent one way to produce a broad range of behaviors. In

their recent, very valuable review of the literature on anomalous diffusion, Metzler and Klafter [1] have drawn attention to possible interpretations of a model that arises naturally from a long-time limit of a continuous-time random walk with nonclassical but uncoupled spatial and temporal statistics. If  $p(\mathbf{r}, t)$  denotes the probability density function associated with  $\mathbf{R}(t)$ , the canonical, two-exponent model for motion in unbounded  $d$ -dimensional Euclidean space corresponds (with  $0 < \alpha \leq 2$ ,  $0 < \beta > 1$ , and  $K_\alpha$  a constant) to

$$p^*(\mathbf{q}, u) = [u^{\beta-1}/(u^\beta + K_\alpha |\mathbf{q}|^\alpha)] \tilde{p}(\mathbf{q}, 0), \quad (1)$$

where we have introduced the spatial Fourier transform

$$\tilde{f}(\mathbf{q}) = \mathcal{F}\{f(\mathbf{r}); \mathbf{r} \mapsto \mathbf{q}\} = \int e^{i\mathbf{q} \cdot \mathbf{r}} f(\mathbf{r}) d^d \mathbf{r},$$

the temporal Laplace transform

$$\hat{g}(u) = \mathcal{L}\{g(t); t \mapsto u\} = \int_0^\infty e^{-ut} g(t) dt,$$

and the joint Fourier-Laplace transform

$$h^*(\mathbf{q}, u) = \int_0^\infty e^{-ut} \tilde{h}(\mathbf{q}, t) dt = \int e^{i\mathbf{q} \cdot \mathbf{r}} \hat{h}(\mathbf{r}, u) d^d \mathbf{r}.$$

From the isotropy in  $\mathbf{q}$  of  $p^*(\mathbf{q}, u)$ , it follows that  $p(\mathbf{r}, t)$  is isotropic in  $\mathbf{r}$ . As  $\langle |\mathbf{R}(t)|^2 \rangle \geq \langle |\mathbf{R}(t)| \rangle^2 \geq |\langle \mathbf{R}(t) \rangle|^2$ , the assumption that  $\langle |\mathbf{R}(t)|^2 \rangle < \infty$  yields  $\langle \mathbf{R}(t) \rangle = \mathbf{0}$  and,

$$\mathcal{L}\{\text{Var}\{\mathbf{R}(t)\}; t \mapsto u\} = -\tilde{\nabla}^2 p^*(\mathbf{q}, u)|_{\mathbf{q}=\mathbf{0}},$$

where  $\tilde{\nabla}$  denotes the gradient operator with respect to  $\mathbf{q}$ . The answer is finite if and only if  $\alpha = 2$ , and in this case  $\mathcal{L}\{\text{Var}\{\mathbf{R}(t)\}; t \mapsto u\} \propto u^{-1-\beta}$  as  $u \rightarrow 0$ , so that  $\text{Var}\{\mathbf{R}(t)\} \propto t^\beta$  as  $t \rightarrow \infty$ . The canonical model (1) fails to produce moderate superdiffusive behavior with  $1/2 < \nu < \infty$ , a defect that can be remedied by nontrivial coupling of the interstep times and step lengths.

We can rewrite Eq. (1) in the form

$$u p^*(\mathbf{q}, u) - \tilde{p}(\mathbf{q}, 0) = -K_\alpha u^{1-\beta} |\mathbf{q}|^\alpha p^*(\mathbf{q}, u). \quad (2)$$

The left-hand side is the joint Fourier-Laplace transform of  $\partial p/\partial t$ . Concerning the right-hand side, one may first observe that so long as  $0 < \beta \leq 1$ , for any function  $\phi$  with Laplace transform  $\hat{\phi}$ ,

$$\mathcal{L}^{-1}\{u^{1-\beta}\hat{\phi}(u); u \rightarrow t\} = \frac{1}{\Gamma(\beta)} \frac{\partial}{\partial t} \int_0^t \frac{\phi(t') dt'}{(t-t')^{1-\beta}},$$

and so the evolution equation becomes

$$\frac{\partial p}{\partial t} = -\mathcal{F}^{-1}\left\{\frac{K_\alpha}{\Gamma(\beta)} \frac{\partial}{\partial t} \int_0^t |\mathbf{q}|^\alpha \tilde{p}(\mathbf{q}, t') dt'; \mathbf{q} \rightarrow \mathbf{r}\right\}. \quad (3)$$

In the simplest special case  $\alpha=2$ , this reduces to a result found by Metzler and Klafter [1], namely,

$$\frac{\partial p}{\partial t} = \nabla^2 \left\{ \frac{K_2}{\Gamma(\beta)} \frac{\partial}{\partial t} \int_0^t p(\mathbf{r}, t') dt' \right\}.$$

If  $\beta=1$  also, the integral operator becomes trivial and the familiar diffusion equation

$$(\partial p/\partial t) = D \nabla^2 p \quad (4)$$

is recovered, with  $D=K_2$  the usual diffusion constant. Keeping  $\beta < 1$  retains the prospect of subdiffusion.

Metzler and Klafter [1] discuss all these matters in terms of fractional integral operators. Their viewpoint emerges from their study of a large body of work based on variants of the radially symmetric diffusion equation. To obtain a real-space evolution equation, Metzler and Klafter propose the use of fractional integral operators over space. This strategy, while mathematically acceptable, breaks the symmetry of the process, and there are tiresome complications with noninteger powers of  $e^{i\pi/2}$ .

In the subsequent discussion it will suffice to restrict our attention to the inversion of the Fourier transform in the case  $\beta=1$ , since the extension of the analysis to cover  $\beta < 1$  is so straightforward. We thus have to analyze

$$(\partial p/\partial t) = -K_\alpha \mathcal{F}^{-1}\{|\mathbf{q}|^\alpha \tilde{p}(\mathbf{q}, t); \mathbf{q} \rightarrow \mathbf{r}\}. \quad (5)$$

This is actually a classic problem in the theory of the stable distributions of Lévy, but the existing discussions are disappointingly incomplete [11–15].

If we make only the assumption that probability has to be transferred continuously across surfaces via a flux vector  $\mathbf{j}$ , rather than disappearing at one point and reappearing at a distant point, we are led to the *continuity equation*

$$(\partial p/\partial t) + \nabla \cdot \mathbf{j} = 0.$$

At this level in the modeling, the detailed nature of the relation between flux vector  $\mathbf{j}$  and probability has not been used. For classical modeling, one usually assumes *Fick's law*  $\mathbf{j} = -D \nabla p$ , which asserts that the diffusing substance moves to destroy concentration gradients (here, equivalently, probability gradients) and we arrive at the classical diffusion equation (4). Since the Fourier transform of the gradient op-

erator  $\nabla$  produces a factor  $-i\mathbf{q}$ , we can only rewrite Eq. (5) as a continuity equation if we define the Fourier transform of the flux vector to be

$$\mathbf{j}(\mathbf{q}, t) = K_\alpha i \tilde{p}(\mathbf{q}, t) |\mathbf{q}|^{\alpha-2} \mathbf{q}. \quad (6)$$

It is natural to try to bring  $\nabla p$  into the calculation, not only by analogy with normal diffusion, but also because the only coordinate-free way to introduce space derivatives of  $p$  into the problem and produce a vector result that scales linearly with  $p$  is via  $\nabla p$ . Identifying the right-hand side of Eq. (6) as the transform of a convolution, we arrive at the flux equation

$$\mathbf{j}(\mathbf{r}, t) = -K_\alpha \int \Phi_{\alpha,d}(\mathbf{r}-\mathbf{r}') \nabla p(\mathbf{r}', t) d^d \mathbf{r}', \quad (7)$$

where

$$\Phi_{\alpha,d}(\mathbf{r}) = [1/(2\pi)^d] \int e^{i\mathbf{q}\cdot\mathbf{r}} |\mathbf{q}|^{\alpha-2} d^d \mathbf{q}. \quad (8)$$

As the volume element in spherical polar coordinates scales as  $|\mathbf{q}|^{d-1}$ , this integral fails to exist in the classical sense due to divergence at the origin when  $d+\alpha \leq 2$ , while decay of the integrand at infinity in the polar coordinate integration is lost when  $d+\alpha \geq 3$ . A classical analytical approach is, therefore, necessarily restricted to  $2-d < \alpha < 3-d$ , and even then may be unpleasant due to delicate conditional convergence of the integral (8), which presents difficulties with the use of the convolution formula.

We avoid these problems by working within the Lighthill-Temple theory of generalized functions, guided for  $d=1$  by the brilliant but underused text of Lighthill [16]. For  $d=1$ , the continuity equation reduces to

$$\frac{\partial}{\partial t} p(x, t) + \frac{\partial}{\partial x} j(x, t) = 0, \quad (9)$$

and we need to determine the kernel

$$\Phi_{\alpha,1}(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i\omega x} |\omega|^{\alpha-2} d\omega,$$

to use in the one-dimensional case of Eq. (8). From Lighthill's table (p. 43 of Ref. [16]) we have the formulas

$$\int_{-\infty}^{\infty} e^{-2\pi i x y} |x|^\alpha dx = \frac{2 \cos[\frac{1}{2} \pi(\alpha+1)] \Gamma(\alpha+1)}{(2\pi|y|)^{\alpha+1}}, \quad (10)$$

for  $\alpha \neq 0, \pm 1, \pm 2, \dots$ , and

$$\int_{-\infty}^{\infty} e^{-2\pi i x y} x^{-1} \operatorname{sgn}(x) dx = -2\{\ln|y| + C\}, \quad (11)$$

where  $C$  is an arbitrary constant [17]. We deduce that

$$\Phi_{\alpha,1}(x) = \frac{\cos[\frac{1}{2} \pi(\alpha-1)] \Gamma(\alpha-1)}{\pi|x|^{\alpha-1}}, \quad \alpha \neq 1, \quad (12)$$

$$\Phi_{1,t}(x) = - (1/\pi)\{\ln|x| + \text{const}\}. \quad (13)$$

The case  $d=1$  and  $\alpha=1$ . As  $\int_{-\infty}^{\infty} \partial p/\partial x dx=0$ , the assignment of the arbitrary constant becomes irrelevant, and we have

$$j(x,t) = \frac{K_1}{\pi} \int_{-\infty}^{\infty} \ln|x-y| \frac{\partial}{\partial y} p(y,t) dy. \quad (14)$$

Although derived by the use of generalized functions, this formula admits a sensible interpretation as an ordinary integral. Equations (9) and (14) constitute an evolution equation for the  $\alpha=1$  stable distribution that appears to be new [18], and has more physical appeal than the previously derived evolution equation

$$(\partial^2 p/\partial t^2) + K_1^2 (\partial^2 p/\partial x^2) = 0, \quad (15)$$

discussed by Medgyessy [19], which does not admit a simple flux interpretation.

A classical and fully rigorous verification of the correctness of the evolution equation may be carried out as follows. The stable distribution defined by  $\tilde{p}(q,t) = \exp(-K_1 t|q|)$  corresponds in real space to the Cauchy density or Lorentzian packet

$$p(x,t) = (K_1 t/\pi)[x^2 + (K_1 t)^2]^{-1}. \quad (16)$$

A little algebra shows that the corresponding flux predicted by the formula (14) is

$$j(x,t) = - \frac{2K_1^2 t}{\pi^2} \int_0^{\infty} \ln z \left\{ \frac{z+x}{[(z+x)^2 + (K_1 t)^2]^2} - \frac{z-x}{[(z-x)^2 + (K_1 t)^2]^2} \right\} dz.$$

The integral can be evaluated by noting that for any rational function  $Q(z)$  that is free from poles on the non-negative real axis and is  $O(z^{-2})$  as  $z \rightarrow \infty$ ,

$$\int_0^{\infty} Q(z) \ln z dz = \frac{1}{2} \sum \text{Res}\{Q(-z)(\ln z)^2\},$$

where the complex logarithm is given its principal value (so that  $-\pi < \arg z \leq \pi$ ), and the predicted flux for the Cauchy density becomes, after some algebra,

$$j(x,t) = (K_1 x/\pi)[x^2 + (K_1 t)^2]^{-1}. \quad (17)$$

The density (16) and flux (17) are easily verified to be consistent with the continuity equation (9), and the proof that the  $\alpha=1$  evolution law is correct is complete.

The case  $d=1$  when  $1 < \alpha < 2$ . Here the flux becomes

$$j(x,t) = -K_\alpha \int_{-\infty}^{\infty} \Phi_{\alpha,1}(x-y) \frac{\partial}{\partial y} p(y,t) dy, \quad (18)$$

where the kernel  $\Phi_{\alpha,1}(x-y)$  is given by Eq. (12). For  $1 < \alpha < 2$ , the kernel has an integrable singularity at  $y=x$ , is

always positive, and decays as  $|x-y|$  increases. The flux at  $x$  samples the current probability gradient throughout all space, with greatest weight in the neighborhood of  $x$ , but significant contributions from remote points. The evolution equation can be written in the form

$$\frac{\partial}{\partial t} p(x,t) = K_\alpha \frac{\partial}{\partial x} \int_{-\infty}^{\infty} \Phi_{\alpha,1}(x-y) \frac{\partial}{\partial y} p(y,t) dy. \quad (19)$$

Medgyessy [14], in Appendix 6 of his paper, has given an alternative evolution equation for  $1 < \alpha < 2$  that does not exhibit a flux and does not reveal the underlying continuity equation. His equation, rewritten in the notation of the present paper, is

$$\frac{\partial}{\partial t} p(x,t) = K_\alpha \int_{-\infty}^{\infty} \Phi_{\alpha,1}(x-y) \frac{\partial^2}{\partial y^2} p(y,t) dy. \quad (20)$$

One can formally pass from Medgyessy's evolution equation to Eq. (19) by one integration by parts, and the use of the identity

$$(\partial/\partial x)\Phi_{\alpha,1}(x-y) = -(\partial/\partial y)\Phi_{\alpha,1}(x-y),$$

but this step is invalid since the differentiated kernel has a nonintegrable divergence at  $y=x$ . However, we could have arrived at Medgyessy's form directly from the Fourier analysis by choosing to invert the Fourier transform as a convolution of a kernel with  $\partial^2 p/\partial x^2$ , rather than first extracting a flux.

The case  $d=1$  when  $0 < \alpha < 1$ . As in the preceding case, the flux is given by Eq. (18) where the kernel  $\Phi_{\alpha,1}(x-y)$  is given by Eq. (12). For  $0 < \alpha < 1$ , the kernel is continuous, and its only misbehavior is a cusp at  $y=x$ . It is always negative (the flux thus enhancing rather than opposing concentration gradients) and grows as  $|x-y|$  increases. It is known that for one-dimensional stable processes with  $0 < \alpha < 1$ , the sample paths are almost surely discontinuous at all points. For physical modeling of particle transport processes, where continuity of individual particle trajectories is a physical necessity, models based on stable laws of order  $\alpha < 1$  are highly suspect. Our analysis shows that if one wishes to use them and preserve a flux interpretation of the transport process, the flux has unpleasant features [20].

Medgyessy's evolution equation for  $0 < \alpha < 1$  is (after some gamma function manipulations)

$$\frac{\partial p}{\partial t} = \frac{K_\alpha \Gamma(\alpha-1) \cos[\frac{1}{2} \pi(\alpha-1)]}{\pi} \times (1-\alpha) \int_{-\infty}^{\infty} \frac{\text{sgn}(x-y)}{|x-y|^\alpha} \frac{\partial}{\partial y} p(y,t) dy.$$

Since

$$\frac{(1-\alpha) \text{sgn}(x-y)}{|x-y|^\alpha} = \frac{\partial}{\partial x} |x-y|^{1-\alpha},$$

it is possible to pass by purely classical means from Medgyessy's equation to our flux-based equation simply by extracting an  $x$  derivative from inside the integral.

*Case with  $d > 1$ .* Extending the generalized function ideas to isotropic problems with  $d > 1$  is straightforward. The awkwardness with the special case  $\alpha = 1$  encountered for  $d = 1$  does not arise. One finds [21] that

$$\int \exp(-i\mathbf{q}\cdot\mathbf{r})|\mathbf{q}|^{\kappa}d^d\mathbf{q} = \frac{\Gamma(\frac{1}{2}\kappa + \frac{1}{2}d)}{\Gamma(-\frac{1}{2}\kappa)} \frac{2^{\kappa+d}\pi^{d/2}}{|\mathbf{r}|^{\kappa+d}}.$$

Hence for  $d \geq 2$  and  $0 < \alpha < 2$  we find that

$$\Phi_{\alpha,d}(\mathbf{r}) = \frac{2^{\alpha-2}}{\pi^{d/2}} \frac{\Gamma(\frac{1}{2}[\alpha+d]-1)}{\Gamma(1-\frac{1}{2}\alpha)} |\mathbf{r}|^{2-d-\alpha}.$$

The corresponding integral (7) for the flux is classically convergent for  $0 < \alpha < 2$ , provided that  $p(\mathbf{r},t)$  decays adequately at infinity. Compare this with the result of a classical Fourier analysis treatment, which would require (as noted earlier)  $2 - \alpha < d < 3 - \alpha$ . The kernel  $\Phi_{\alpha,d}(\mathbf{r})$  is always positive, and decays at infinity for all  $d \geq 2$ .

It is suggested that an application of generalized functions from the Lighthill perspective in other areas of stochastic modeling may shed light on other subtle phenomena.

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- $$\partial p / \partial t = D \partial / \partial x \int_{-\infty}^{\infty} \pi^{-1}(x'-x)^{-1} p(x',t) dx'.$$
- [their Eq. (39) with the drift  $\gamma$  set to zero]. The integral has to be interpreted as a Cauchy principal value. This formalism fails to bring out the linear relation between the flux and the probability gradient, and although one can formally obtain Eq. (14) by integrating parts, that operation if naively performed is invalid.
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