Stochastic transport and fractional derivatives

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A systematic derivation of macroscopic equations describing superdiffusion (8) and subdiffusion (20) over a wide range of physical processes is given on the basis of general microscopic characteristics of the motion of individual particles. It is shown that fractional derivatives are a necessary component of these equations, the time derivatives being of a different type from the derivatives with respect to the spatial variables. The simplest properties of the equations are investigated—specifically, how quickly a universal self-similar profile emerges from an arbitrary initial particle distribution. © *1995 American Institute of Physics.*

1. INTRODUCTION

The main objective of this work is to inform the reader of the simple fact that there is no substitute for the mathematical language of fractional derivatives for describing and studying the physical process of stochastic transport. Stochastic transport is now one of the most fashionable and popular fields of physics, making it possible to relate otherwise very disparate phenomena, such as dissipative transport of real particles, heat, light, magnetic fields, and so on, in ordinary space,[1] and the dynamics of point-representations of Hamiltonian mechanical systems in phase space.[2,3] The basis for this is the general and universal property of "forgetting" or "information loss"—the property that characterizes the stochasticity of a process.

In theoretical research on random transport, two methods or levels of description of the motion are ordinarily employed—microscopic and macroscopic. The first method concerns the law of motion of individual particles and the second method concerns an ensemble of particles. The two methods are certainly interrelated, and detailed understaneding of one makes it possible to determine the second—the random walk process is equivalent to the diffusion equation and vice versa,[4] but for various aspects of the phenomena of interest to the investigator in each specific case, one method can be much more convenient than the other. Moreover, in both real experiments and simulations, as a rule, it is impossible to investigate both aspects of the phenomenon at the same time.

For this reason, it is regrettable that the aforementioned duality of the approach to the most popular and classical example of stochastic transport is largely lost in the study of more complicated motions. Indeed, although attempts have been made from time to time to describe systems with power-law random displacements

$$\langle x\rangle \propto t^{\alpha} \tag{1}$$

that have been investigated at the microscopic level in terms of a macroscopic equation, such attempts have not, in general, conformed to a rigorous, systematic approach, as evidenced by the fact that this question is not discussed at all in the excellent reviews in Refs. 1, 4, and 5. In the last few years, it has often been suggested that fractional derivatives be used for such a description (see, for example, Refs. 6 and 7), but they are introduced purely phenomenologically, in fact immediately after writing down Eq. (1). Without a detailed analysis of the motion of individual particles, this leaves the impression that the choice of the language of fractional derivatives is arbitrary and exotic. Moreover, the proposed equations are not even solved, i.e., even the convenience of this language remains unclear.

In the present paper, we present a systematic and rigorous derivation of equations that describe stochastic but nondiffusion ($\alpha \neq 1/2$) spreading of an ensemble of particles, without any preliminary information about fractional derivatives. The terms from this field of mathematics are first used only after such derivatives appear explicitly. The basic properties of the derived equations, which are analyzed below, attest to the extreme simplicity of applying these equations in physical problems, similar to the simplicity and convenience of the classical diffusion equation. All problems are solved in the one-dimensional case (the extension to higher dimensions presents only technical difficulties which can be easily overcome). The derivation is not tied to any specific physical system, and is based on general models of microscopic motion (1), where it has long been a standard procedure, in comparisons with standard diffusion, to distinguish the more rapid superdiffusion ($\alpha > 1/2$) and the slower subdiffusion ($\alpha < 1/2$).[1,4,5] The starting point is a discrete model of classical random transport, in which a particle executes equiprobable hops to the left and right over a distance $\Delta x = 1$ in the time $\Delta t = 1$, such that at macroscopic times and scales ($t \gg 1$, $x \gg 1$) the model yields the diffusion equation for the particle density[4]

$$\frac{\partial n}{\partial t} = \frac{1}{2}\frac{\partial^2 n}{\partial x^2}. \tag{2}$$

For a real physical process (an actual random walker), it is always possible to find appropriate quantities Δx and Δt, which differ from one phenomenon to another, but in the general mathematical approach it is convenient to employ dimensionless quantities. The physical media in which stochastic transport occurs are assumed to be uniform, isotropic, and stationary in the sense that their properties do not change

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in time or space. All simplifications are made for the sake of computational simplicity and clarity. Subsequent generalizations are possible.

2. SUPERDIFFUSION

At the microscopic level, "Levy flights" provide the most faithful mathematical model of fast particles.[1,4,5] Here the discreteness of the hops in time is preserved, but the spatial motion becomes continuous. The spatial motion is characterized by a distribution function $f(x)$, equal to the probability distribution of a displacement at the next hop from a given point to the coordinate x. Therefore $f(x)$ is a nonnegative-definite, even (as a result of the isotropy of the medium) function, which is identical at all points in space (as a result of its uniformity), and $\int_{-\infty}^{+\infty} f(x)dx=1$. Levy flights inherently describe functions with an infinite mean-square displacement:

$$\langle x^2\rangle=\int_{-\infty}^{+\infty} x^2 f(x)dx=\infty. \tag{3}$$

Thus, the outlying "tails" of f, which as a rule are assumed to be power-law functions, are responsible for superdiffusion. In what follows, to bring some degree of definiteness to the numerical coefficients, the following class of functions is used in the intermediate calculations:

$$f(x)=\frac{\Gamma(\beta+1/2)}{\sqrt{\pi}\Gamma(\beta)}\frac{1}{(1+x^2)^{\beta+1/2}}, \quad \beta>0 \tag{4}$$

where $\Gamma(\alpha)$ is the gamma function. Since the final answer depends only on the power-law "tail," it will be universal and identical however different the behavior of various systems (various f) at microscopic scales $x\sim 1$. The "flights" occur for $\beta\leqslant 1$. One physical example of such a process is the transfer of resonance radiation in a tenuous gas (or plasma) (see the Biberman–Holsteĭn equation in Ref. 8): for a Doppler line contour, say, $\beta\simeq 1/2$, and for a Lorentzian contour, $\beta=1/4$.

It is easy to see that the equation describing the dynamics of the particle density for arbitrary f has the form

$$n(x,t+1)-n(x,t)=\int_{-\infty}^{+\infty}[n(x-x',t) -n(x,t)]\, f(x')dx'. \tag{5}$$

Expanding the function $n(x,t)$ (which is continuous at macroscopic times and scales) in a Taylor series in x and t, and noting that $f(x)$ is even, it is easy to see that for finite $\langle x^2\rangle$, Eq. (5) reduces to the diffusion equation with diffusion coefficient $D=\langle x^2\rangle/2$, and in the case (3) it remains an integral equation.

To study this regime in greater detail and to derive the desired mathematical formula, it is convenient to take the Fourier transform with respect to x, which transforms the convolution integral on the right-hand side of Eq. (5) into a product of Fourier transforms

$$\partial n_k/\partial t=(f_k-1)n_k, \tag{6}$$

where for f given by Eq. (4),

$$f_k=\frac{2^{1-\beta}}{\Gamma(\beta)}k^\beta K_\beta(k)$$

and K_β is the modified Bessel function of the second kind. Since the ultimate objective is to derive a macroscopic transport equation describing the motion of a particle ensemble over large scales $x\gg 1$ $(k\ll 1)$, in Eq. (6) f_{k-1} can be expanded in a series near $k=0$, and only the first nonvanishing term need be retained. This yields

$$\frac{\partial n_k}{\partial t}=-\frac{k^2}{[4(\beta-1)]}n_k, \quad \beta>1,$$

$$\frac{\partial n_k}{\partial t}=-\frac{\Gamma(1-\beta)}{\Gamma(1+\beta)}\frac{|k|^{2\beta}}{2^{2\beta}}n_k, \quad \beta<1,$$

$$\frac{\partial n_k}{\partial t}=k^2 n_k\frac{\ln|k|}{2}, \quad \beta=1. \tag{7}$$

In the latter case, dropping the remaining terms obviously leads to an unphysical instability for small scales $(k>1)$; however, this instability can be easily eliminated by introducing any correction (since we are not interested in motion on small scales) that is small for $k\ll 1$ but gives the correct sign for large k. For example, $\ln|k|$ can be replaced with $\ln[|k|/(|k|+1)]$.

The second of Eqs. (7), written in ordinary space as (compare to Eq. (5))

$$\frac{\partial n}{\partial t}=\frac{\Gamma(\beta+1/2)}{\sqrt{\pi}\Gamma(\beta)}P\int_{-\infty}^{+\infty}\frac{n(x')}{|x-x'|^{2\beta+1}}dx' \tag{8}$$

corresponds to superdiffusion. The expression on the right-hand side is a fractional derivative.[9] In multidimensional form, it is a fractional power of the Laplacian Δ^β. It is usually defined in terms of its Fourier transform (7). Naturally, manipulations with it are especially convenient in this representation, where they are technically identical to the case of a classical (local) diffusion operator. The general solution of Eq. (8)

$$n_k(t)=\exp\left[-\frac{\Gamma(1-\beta)}{\Gamma(1+\beta)}\frac{|k|^{2\beta}}{2^{2\beta}}t\right]n_k(0) \tag{9}$$

can be written in ordinary space in the form

$$n(x,t)=\int_{-\infty}^{+\infty}G(x-x',t)n(x',0)dx', \tag{10}$$

where the Green's function of Eq. (8) is self-similar and is equal to

$$G(x,t)=\frac{1}{t^{1/2\beta}}\Phi\left(\frac{x}{t^{1/2\beta}}\right),$$

$$\Phi(\xi)=\frac{1}{\pi}\int_0^\infty \exp\left[-\frac{\Gamma(1-\beta)}{\Gamma(1+\beta)}\frac{\kappa^{2\beta}}{2^{2\beta}}\right]\cos\kappa\xi d\kappa. \tag{11}$$

The Green's function itself can be found from the microscopic description of the process[4,5] (in complete correspondence with the self-sufficiency (but not convenience) of any level of description indicated in the introduction), but the macroscopic approach (10) shows much more clearly, for example, the characteristic property of stochastic transport that in the limit $t \to \infty$, when the profile $G(x)$ beomes very smooth,

$$n(x,t) \to AG(x,t), \quad A = \int_{-\infty}^{+\infty} n(x,0)dx.$$

This emergence into a self-similar (universal) regime is a manifestation of the property of "information loss" in a stochastic process (as compared to the case of the ordinary diffusion equation[10]). It is related to the fact that, as one can see from Eq. (9), in the limit $t \to \infty$, the Green's function "cuts off" all initial harmonics with $k \neq 0$, and that annihilation of overtones is responsible for the asymptotic approach to a universal one-parameter profile. A significant difference from classical diffusion is that the corresponding self-similar profile is not Gaussian, but has instead a power-law "tail":

$$n(x,t)|_{x \to \infty} = A \frac{\Gamma(\beta + 1/2)}{\sqrt{\pi}\Gamma(\beta)} \frac{t}{x^{2\beta+1}}. \qquad (12)$$

(Notably, as $\beta \to 1$, its amplitude and the power of x approach finite values.[4]) This can also be calculated from the inverse Fourier transform (11), i.e., once again starting from the microscopic description,[4,5] but it is simpler to see from the macroscopic equation (8). Indeed, as $x \to \infty$, the power-law kernel can be taken outside the integral, and particle conservation can be invoked:

$$\int_{-\infty}^{+\infty} n(x,t)dx = \text{const} = A,$$

after which Eq. (12) is obtained immediately. Thus, the linear time dependence of the tail is related to the "constancy of the particle flux on large scales"[11] —the finite probability of particles to hop from the "core" of the distribution immediately to the "tail."

It is also interesting to note that the somewhat subtle property of the loss of positive-definiteness of the Green's function (11) for unphysical values $\beta > 1$ can also be easily proved from Eqs. (7) and (8), since by separating out the Laplacian

$$|k|^{2\beta} = -k^2(-|k|^{2\beta-2})$$

the function $|k|^{2\beta}$ with $\beta > 1$ can be transferred into the class of functions with $\beta < 1$, but with a negative sign. Since in ordinary space the operator $\partial^2/\partial x^2$ does not change the sign of a power-law function, after repeating the macroscopic derivation of (12) we immediately find that the tail of G is negative (albeit for $\beta > 2$ we again end up in the region where its values are positive). Even these examples of the mathematical simplifications attest to the usefulness of the macroscopic approach. It can be even more useful in specific physical problems.

In concluding this section, we point out that the convergence of n to a self-similar profile can be improved by introducing one more parametrization—a displacement $G(x - x_0)$: expanding the Green's function in Eq. (10) in a Taylor series in x and writing $\int xn(x,0)dx = Ax_0$, it can be shown that if the integral $\int x^2 n(x,0)dx$ is finite,

$$n(x,t) = AG(x - x_0)[1 + O(t^{-\beta})]. \qquad (13)$$

The case of a Gaussian Green's function is different, in that the next term in the expansion—the initial width $n(x,t)$—can also be compensated by an additional displacement in time $G(t + t_0)$.[10] Here this is not the case: the corresponding operation is possible only if the initial distribution $n(x)$ has a symmetric power-law tail $|x|^{-2\beta-1}$. Moreover, since in this region it is necessary to work with functions with diverging moments, there is no reason to believe that x^2 averaged over $n(x,0)$ will be finite. In general, according to the considerations indicated above, the rate at which the self-similar regime emerges is determined by the behavior of $n_k(0)$ in the limit $k \to 0$: if $n_k(0) = A + iAx_0 k + C|k|^{\delta} + \ldots$ with $\delta < 2$, then the correction term in Eq. (12) will decrease as $O(t^{-\delta\beta/2})$.

3. SUBDIFFUSION

"Traps" provide the most faithful microscopic model of slow stochastic particle transport; these appears to have first been proposed in Ref. 12 (see also Refs. 1, 4, and 5). Here, the spatial hops are discrete and the temporal dynamics is continuous; specifically, there exists a distribution function $f(t)$ which is equal to the probability distribution of hops occurring to neighboring points within a time t after the initial point is reached. It is nonnegative-definite, it does not depend on x, and $\int_0^\infty f(t)dt = 1$. The concept of a "trap" corresponds to an infinite mean expectation transition time,

$$\langle t \rangle = \int_0^\infty tf(t)dt = \infty. \qquad (14)$$

The power-law tail of f is therefore responsible for subdiffusion (compare the preceding section), and to make specific calculations, in what follows we choose f to be of the form

$$f(t) = \frac{1}{\gamma} \frac{1}{(1+t)^{\gamma+1}}, \quad \gamma > 0. \qquad (15)$$

Traps appear for $\gamma \leq 1$. A physical example here is charge transport in amorphous materials,[4,5] where $\gamma \simeq 1/2$.

The calculations for this regime are more complicated than for superdiffusion. Since the particles located at a given point in space "remember" well when they arrived at that point, here it is necessary to introduce a characteristic time τ (time of arrival at the point) and particle density distribution N at a given point over this time:

$$n(x,t) = \int_0^\infty N(x,t,\tau)d\tau.$$

It is also convenient to use a different notation for the probability that the particles "survive" (i.e., do not hop to neighboring points) to time τ:

$$F(\tau) = 1 - \int_0^\tau f(t)dt = \frac{1}{(1+\tau)^\gamma}.$$

In these terms

$$n(x,t) = \frac{1}{2} \int_0^t [Q(x-1, t-\tau) + Q(x+1, t-\tau)]F(\tau)d\tau$$

$$+\int_t^\infty \frac{N_0(x,\tau-t)}{F(\tau-t)} F(\tau)d\tau,$$

$$Q(x,t)=\int_0^\infty \frac{N(\tau)}{F(\tau)} f(\tau)d\tau. \tag{16}$$

Here $Q(x,t)$ is the particle flux from a given point to neighboring points (the factor 1/2 results from the fact that the probability of a hop to the right is equal to the probability of a hop to the left), and $N_0(x,\tau)$ is the initial distribution function at the given point (initial condition). Next, for simplicity (see Introduction) we assume that $N_0=n_0(x)\delta_+(\tau)$, where δ_+ is the "shifted" Dirac delta function with the normalization condition $\int_0^\infty \delta_+(\tau)d\tau=1$. It then follows from Eq. (15) that

$$n(x,t)-\int_0^t n(x,t-\tau)f(\tau)d\tau=\frac{1}{2}\int_0^t[n(x-1,\,t-\tau)$$
$$+n(x+1,\,t-\tau)-2n(x,t-\tau)]\,f(\tau)d\tau$$
$$+n_0(x)F(t), \tag{17}$$

which, after $n(x,t)$ is expanded in a Taylor series at macroscopic times and scales, reduces at finite $\langle\tau\rangle$ to the diffusion equation with $D=1/(2\langle\tau\rangle)$ (the integral operator on the right-hand side is replaced by 1), and in the case of Eq. (14) it remains an integral equation.

Here it is convenient to employ an integral transform, as in the superdiffusion regime—but now the Laplace transform, not the Fourier transform, and in time, not space. Then it follows from Eq. (17) that

$$\frac{pF_p}{1-pF_p}n_p=\frac{1}{2}\frac{d^2n_p}{dx^2}+\frac{F_p}{1-pF_p}n_0, \tag{18}$$

where, according to Eq. (15),

$$pF_p=p^\gamma e^p\Gamma(1-\gamma,p)$$

($\Gamma(a,b)$ is the complement of the incomplete gamma function). In the desired macroscopic description, only values $p\ll 1$ are important, and Eq. (18) reduces to

$$\frac{p}{\gamma-1}n_p=\frac{1}{2}\frac{d^2n_p}{dx^2}+n_0/(\gamma-1),\quad \gamma>1,$$

$$\Gamma(1-\gamma)p^\gamma n_p=\frac{1}{2}\frac{d^2n_p}{dx^2}+\Gamma(1-\gamma)p^{\gamma-1}n_0,\quad \gamma<1,$$

$$-p\ln pn_p=\frac{1}{2}\frac{d^2n_p}{dx^2}-\ln pn_0,\quad \gamma=1. \tag{19}$$

The subdiffusion regime describes a second variant which has the following form in the physical coordinates (compare Eq. (17))

$$\frac{\partial}{\partial t}\int_0^t \frac{n(x,t')}{(t-t')^\gamma}dt'=\frac{1}{2}\frac{\partial^2 n}{\partial x^2}+\frac{n_0(x)}{t^\gamma}, \tag{20}$$

which is the desired equation. The left-hand side contains the fractional derivative $\partial^\gamma/\partial t^\gamma$,[9] but of a different type than in the preceding section. Generally speaking, the extension of differential operators to fractional powers can be made by various methods, and the Fourier and Laplace transform languages employed here give different expressions (other variants are also known in mathematics[9]). This asymmetry of the spatial and temporal variables in physics is not surprising, since it is a manifestation of the causality principle. The rigorous derivation of the macroscopic equations which was presented in the present paper automatically takes into account this simple circumstance—in contrast to the phenomenological approach in Ref. 6, where it was proposed that the same types of fractional derivatives in x and t (of the type (20)) be used to describe nondiffusion stochastic processes.

Moreover, in Refs. 6 and 7, because of the qualitative nature of the arguments employed there, the last term on the right-hand side of Eq. (20), whose role is by no means merely formal—since it is responsible, for example, for the nonequivalence of systems with the same values of α discussed in the concluding section—dropped out of the corresponding equations.

It is no more difficult to perform operations with Eq. (20) that to perform similar operations with Eq. (8). After Fourier transforming with respect to x, its solution assumes the form

$$n_{pk}=\frac{2\Gamma(1-\gamma)p^{\gamma-1}}{2\Gamma(1-\gamma)p^\gamma+k^2}n_{0k},$$

which in physical variables once again looks like Eq. (10) with a self-similar Green's function (compare the derivation based on the microscopic description,[13])

$$G(x,t)=\frac{1}{t^{\gamma/2}}\Phi\left(\frac{x}{t^{\gamma/2}}\right),$$

$$\Phi(\xi)=\frac{\sqrt{2\Gamma(1-\gamma)}}{2\pi i\gamma}\int \exp\,[z^{2/\gamma}-\sqrt{2\Gamma(1-\gamma)}|\xi|z]dz, \tag{21}$$

where the integral in the complex z plane extends over a contour running from the fourth quadrant into the first quadrant consisting of two rays at polar angles $\varphi=\pm\pi\gamma/4$. As $|\xi|\to\infty$, deforming this contour and passing it through the saddle point

$$z=\left[\frac{\gamma}{2}\sqrt{2\Gamma(1-\gamma)}\left|\xi\right|\right]^{\gamma/(2-\gamma)},$$

we obtain (compare Ref. 13)

$$\Phi(\xi)\propto|\xi|^{(\gamma-1)(2-\gamma)}\exp\left[-\frac{2-\gamma}{\gamma}\right.$$
$$\left.\times\left(\frac{\gamma^2}{2}\Gamma(1-\gamma)\xi^2\right)^{1/(2-\gamma)}\right].$$

In this variant of stochastic transport, we are once again dealing with emergence into a self-similar regime

$$n(x,t)=AG(x-x_0,t)[1+O(t^{-\gamma})],$$

for which, as before, in the general case the convergence cannot be improved by shifting the origin of the time t (though, as one can see from the preceding discussion, the moments of G are finite here).

4. CONCLUSION

It has been shown in this paper that in a systematic macroscopic description of stochastic processes, one must deal in a definite order with equations containing fractional derivatives, the derivatives being different in the super and subdiffusion variants—Eq. (8) and (20), respectively. It is no more difficult to work with these equations than with the standard diffusion equation, since the integral terms become local as a result of Fourier and Laplace transforms. The proposed method admits very simple and clearly understandable generalizations to multidimensional cases and the presence of combined spatial and temporal "blurring" of the hops. We merely note here the curious inequivalence of physical processes (characterized simultaneously by Eqs. (4) and (15)) with the same value of α (i.e., identical self-similarity) but different β and γ. For example, stochastic transport with $\alpha=\beta=\gamma=1/2$ is not classical diffusion. For such processes the Green's function (and, therefore, the asymptotic solution) has different power-law "tails" $t^{\gamma}/|x|^{2\beta+1}$ in the limit $|x|\rightarrow\infty$.[6] The most direct and clear way to see this is to repeat the derivation of (12) in the general case (the fractional derivative with respect to t of a power-law function is trivial to obtain and was calculated by Euler[9]). The apparent contradiction with the fact that the repeated application of the operation $\partial^{1/2}/\partial t^{1/2}$ to the equation

$$\frac{\partial^{1/2}n}{\partial t^{1/2}}=\Delta^{1/2}n$$

should transform this equation into Eq. (2) is removed by the presence of the term $(n_0/t^{1/2})$ on the right-hand side, which prevents such a transformation (compare the preceding section)—another argument in favor of a rigorous derivation of the equations.

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