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Memory Effects in Stochastic Transport

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The memory effects in stochastic transport, namely, the dependence of the form of transport equations on the macroscopic time are considered. Equations explicitly taking into account the microscopic aspect of the problem, without which the transfer processes cannot be adequately described, are derived; the methods of their solution are suggested; and the asymptotic properties of the latter are analyzed. © *2003 MAIK "Nauka/Interperiodica".*

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In recent years, growing interest has been shown in the processes of stochastic transport because of the spatial and temporal nonlocalities inherent in this phenomenon [1–4]. The use of an adequate mathematical language of fractional derivatives [5, 6] and stable distributions [1, 7] allowed the physical theory of random transport to be substantially generalized, as compared to the primitive diffusion picture.

There are many physical reasons that are responsible for the above-mentioned nonlocalities (fractional derivatives) in the transport equations (see discussion in [8, 9]). One of the most frequently occurring phenomena is the presence of slowly damping spatial and time correlations in the motion of individual particles in a spreading cloud. Inasmuch as the macroscopic (for cloud) transport equations are derived from the random walk model for individual (not necessarily physical) particles, these equations basically have an asymptotic character. In our preceding work [8], concerning the effects caused by the limited walk rate, we drew attention to the nontriviality of this asymptotic transition and to the nontrivial dependence of the macroscopic transport on the microscopic details and on the initial conditions. It is our purpose to reveal, in this work, the details of the physical consequences of this ideological and mathematical nontriviality.

Evidently, one should expect that evolution is continuous for any physical process satisfying the causality principle: if the solution to the equations is functionally related to the initial state by the Green's function G_t, i.e., if $n(x, t) = G_{t} * n(t = 0)$, then

$$G_{t_1 + t_2} * n(t = 0) = G_{t_2} * n(t = t_1) = G_{t_2} * (G_{t_1} * n(t = 0)). \quad (1)$$

In other words, if we consider the state at any time t_1 as a new initial condition, we do not disturb the evolution continuity. Nevertheless, the equations discussed in all available works devoted to the nonlocal nondiffusion transport with a fractional time derivative, including a recent excellent review [4], strictly speaking, do not possess this property. This unpleasant fact has in no way been discussed in the literature, though it is precisely the point that is expected to be helpful in the recognition of a hidden defect of the above-mentioned description, namely, of the incompleteness in the description of a particle cloud only in terms of its macroscopic concentration $n(x, t)$. Interestingly, similar problems arise for strongly coupled coulombic systems in the quantum kinetic theory, where the solutions show a strong dependence on the initial correlations [10].

An attempt to unravel this phenomenon leads to the paradoxical conclusion that, even in the cases where the effective equation for macroscopic evolution reduces to the classical diffusion equation containing the familiar first-order time derivative (evidently, satisfying Eq. (1)), the defect is often "hidden under the rug." In reality, the time for approaching the microscopic evolution regime strongly depends on the initial condition and can be much longer than the microscopic time $\langle\tau\rangle$ characterizing the random walk of individual particles (see below). This is especially characteristic of the subdiffusion time operators.

Therefore, the memory effects considered in this work consist not in the familiar temporal nonlocality (fractional derivative) in the effective transport equation but in the fact that the form of this equation depends on the macroscopic time t (see below).

When deriving the transport equations, we will use, as in [6, 8], the standard random walk model. A one-dimensional motion of a particle along the x axis obeys the probability laws $g(|x|)$ and $f(t)$: a particle appearing at any point (say, x_0) may undergo an instantaneous jump to the neighboring points in such a way that the probability of finding it in the interval $(x_0 + x, x_0 + x + dx)$ equals $g(x)dx$, and this transfer proceeds after some waiting process, so that the probability of escaping the

particle residence in the interval $(t, t + dt)$ is equal to $f(t)dt$. For the convenience of intermediate calculations, we choose, without loss of generality, these functions in the form [6, 8]

$$g(x) = \frac{\Gamma(\beta + 1/2)}{\sqrt{\pi}\Gamma(\beta)} \frac{1}{(1 + x^2)^{\beta + 1/2}}; \quad f(t) = \frac{\gamma}{(1 + t)^{\gamma + 1}}. \tag{2}$$

Here, Γ is the Euler gamma function, and the numerical coefficients are determined by the unity normalization condition for g and f. The exponents of the power-law "tails" parameterized by the positive indices β and γ are only essential for further consideration.

The particles at point x "remember" their time of arrival at this point, so that their spatial density n is the integral of a certain distribution N over the "lifetime" τ:

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

Let us define the transition to the subsequent motion in terms of "probability of surviving to time τ," which is simply related to the function f as

$$F(\tau) = 1 - \int_0^\tau f(t)dt.$$

Then, the particle flux $Q(x, t)$ leaving (on both sides and at all distances) a given point can be expressed using the formula for the conditional probability (see [6])

$$Q(x, t) = \int_0^\infty \frac{N(x, t, \tau)}{F(\tau)} f(\tau)d\tau. \tag{3}$$

We can now write the balance equations for the particle at a given time and a given point:

$$n(x, t) = \int_{-\infty}^{+\infty} g(x')\int_0^t Q(x - x', t - t')F(\tau')dt'dx' + \int_t^\infty \frac{N_0(x, \tau - t)}{F(\tau - t)}F(\tau)d\tau. \tag{4}$$

The last term on the right-hand side of this equation accounts for the effect of initial particle lifetime distribution $N_0(x, \tau) \equiv N(x, 0, \tau)$. The set of Eqs. (3) and (4) completely describes the situation and, obviously, satisfies condition (1). Note that, if $N_0 = n_0\delta_+(\tau)$ ("shifted" Dirac delta function: $\int_0^\infty \delta_+(\tau)d\tau = 1$), then, after the arrival of new particles at each point (at any $t > 0$), the self-similar profile

$$N(t, \tau) = \theta(t - \tau)P(t - \tau)F(\tau) \tag{5}$$

forms instantaneously with the correlated dependence on t and τ, where P is the incoming flux and $\theta(t)$ is the Heaviside step function. In this case, one can pass from the set of Eqs. (3) and (4) to a single basic equation for the macroscopic density n [6]:

$$n(x, t) = \int_{-\infty}^{+\infty} g(x') \times \int_0^t f(t')n(x - x', t - t')dt'dx' + F(t)n_0(x). \tag{6}$$

The Green's function of this equation reads

$$G_{k, p} = \frac{F_p}{1 - f_p g_k}, \tag{7}$$

where the symbol $[\cdot]_{k, p}$ denotes the Fourier and/or Laplace component of the corresponding function.

The transport equation can also be written in terms of only n if $f = \mu\exp(-\mu t)$ ($\mu = 1/\langle\tau\rangle$); then F and f (and, hence, Q and n) are proportional to each other. The reason for setting off the exponential law is quite clear, because only in this case does a fixed percentage of the sitting particles leave the point, irrespective of the time of their arrival at this point; i.e., all particles $\int_0^\infty N(\tau)d\tau$ in a "common bag" are in the same conditions. In all other cases, the "reel game" depends on the waiting time τ, and one cannot ignore the details of the $N(\tau)$ distribution.

In the majority of works, Eq. (6) is written without any substantiation, which should imply that either one of the two above-mentioned conditions is fulfilled or a certain model is used (the authors of those works did not discuss this issue). In the general case, Eq. (6) is valid only for a certain asymptotic meaning: a time must be elapsed (see below) until the self-similar dependence (5) covers the larger part of the $N(\tau)$ profile and becomes dominating Q, as compared to N_0. One can readily verify that condition (1) is met for Eq. (6) only if $f = \mu\exp(-\mu t)$. In all other cases, one should use the initial set of Eqs. (3) and (4) to adequately describe the transport process. In what follows, we propose a method for solving this set exactly and show that the initial particle lifetime distribution influences the subsequent evolution.

To begin with, it is convenient to divide $N(x, t, \tau)$ into two terms (see Eq. (4)):

$$N_1(x, t, \tau) = \frac{N_0(x, \tau - t)F(\tau)}{F(\tau - t)}\theta(\tau - t); \tag{8}$$

$$N_2(x, t, \tau) = \int_{-\infty}^{+\infty} g(x')F(\tau)Q(x - x', t - \tau)\theta(t - \tau)dx', \quad \tau < t. \tag{9}$$

The term N_1 describes the particles living at the time point $\tau > t$, i.e., those particles of the initial distribution N_0 which survived up to time t. The term N_2 is the particle profile formed by the flux $Q(x, t)$, to which both N_1 and N_2 make a contribution. The equation for N_2 is analogous to Eq. (4) and follows from Eq. (3) for the flux:

$$\begin{aligned} &N_2(x, t, \tau) \\ &= F(\tau)\int_{-\infty}^{+\infty} g(x')\left\{\int_0^{t-\tau}\frac{N_2(x-x', t-\tau, \tau_1)f(\tau_1)}{F(\tau_1)}d\tau\right. \\ &\left.+\int_{t-\tau}^{+\infty}\frac{N_1(x-x', t-\tau_1, \tau_1)f(\tau_1)}{F(\tau_1)}d\tau\right\}dx'. \end{aligned} \quad (10)$$

Let us substitute Eqs. (8) and (9) in Eq. (10) and perform the Laplace and Fourier transforms with respect to time and spatial variables, respectively, to get rid of convolution integrals. After this, we again use Eq. (9) and set off the term $N_{2p,k}$ on the right-hand side of the resulting expression. By solving the linear equation for this term, we get

$$\begin{aligned} N_{2p,k}(\tau) &= \frac{g_k F(\tau)\exp(-p\tau)}{1-f_p g_k} \\ &\times\left(\int_t^{+\infty}\frac{N_{0k}(\tau_1-t)f(\tau_1)d\tau_1}{F(\tau_1-t)}\right)_p. \end{aligned} \quad (11)$$

The particle density can also be written as the sum of two terms $n = n_1 + n_2$, where

$$n_1 = \int_t^{\infty} N_1(x, t, \tau)d\tau, \quad n_2 = \int_0^t N_2(x, t, \tau)d\tau.$$

Since N_2 depends on its variables in the self-similar manner (9) (cf. Eq. (5)), we can write

$$n_{2p,k} = \frac{F_p N_{2p,k}}{F(\tau)\exp(-p\tau)}. \quad (12)$$

Now, using Eqs. (8) and (11) and the relationship $f_p(t + t') = F(t') - pF_p(t + t')$ (hereafter, the index p denotes the Laplace transform with respect to t), we obtain, after simple mathematics,

$$\begin{aligned} n_{p,k} &= \frac{1}{1-f_p g_k} \\ &\times\left\{F_p n_{0k} + (1-g_k)\int_0^{\infty} N_{0k}(\tau)\left(\frac{F(\tau+t)}{F(\tau)} - F(t)\right)_p d\tau\right\}. \end{aligned} \quad (13)$$

Note that the first term in braces is the solution to Eq. (6) for the density (see [6]), and, hence, the second term demonstrates the dependence of the solution on the initial lifetime distribution. Note again that the second term becomes zero for $F(t) = \exp(-\mu t)$; i.e., the dependence on the microscopic distribution vanishes.

To demonstrate the distinctions between Eqs. (13) and (6), we consider an example with the initial condition $N_0(x, \tau) = n_0(x)\delta_+(\tau - t_0)$, where t_0 is a certain nonnegative delay time. In this case, the solution can be written in a different and more compact form. By substituting the initial condition into Eq. (11) and using Eq. (12), we obtain

$$n_{2p,k} = \frac{g_k}{F(t_0)}\frac{F_p n_{0k}}{1-f_p g_k} f_p(t + t_0),$$

$$n_1 = \frac{F(t + t_0)n_0(x)}{F(t_0)}.$$

Finally, we write the expression for the particle density $n(x, t)$

$$\begin{aligned} n(x, t) &= \frac{1}{F(t_0)}\left(\int_{-\infty}^{+\infty} dx' g(x')\right. \\ &\left.\times\int_0^t f(\tau + t_0)\tilde{n}(x-x', t-\tau)d\tau + F(t + t_0)n_0(x)\right), \end{aligned}$$

where $n(x, t)$ stands for the already known solution to Eq. (6), towards which $\tilde{n}(x, t)$ tends at large t's. However, the initial stage of density evolution at $t < t_0$, which, depending on t_0, can be rather prolonged, proceeds in a different way. For clearness, let us consider the situation with $\beta, \gamma > 1$. In this case, the function f has a nonzero first moment $\langle\tau\rangle$ (mean waiting time) and the function g has a finite or noninfinite second moment $\langle x^2\rangle$ (mean square displacement). Hence, after expanding the integrand in Eq. (6) with allowance for the smallnesses $t \gg \langle\tau\rangle$ and $x \gg \sqrt{\langle x^2\rangle}$, we should arrive at the standard diffusion equation with the coefficient $D = \langle x^2\rangle/2\langle\tau\rangle$. In our situation, this is not the case. After expanding the expression for n_1 in powers of the small parameter $t/t_0 \ll 1$, we see that the number of such particles decreases linearly with time following the law

$$n_1(x, t) \simeq n_0(x)(1 - \gamma t/t_0), \quad (14)$$

which leads, correspondingly, to a linear increase in the number of particles n_2, so that the evolution of density n_2 at $t \gg \langle\tau\rangle$ obeys the diffusion equation with a constant source on the right-hand side:

$$\begin{aligned} &\frac{\partial n_2}{\partial t} = D\frac{\partial^2 n_2}{\partial x^2} + \varphi(x); \\ &\varphi(x) = \frac{\gamma}{t_0}\int_{-\infty}^{+\infty} g(x')n_0(x-x')dx', \quad D = \frac{\langle x^2\rangle}{2\langle\tau\rangle}. \end{aligned} \quad (15)$$

Its solution has the form (see, e.g., [11])

$$n_2(x, t) = \int_0^{t} \int_{-\infty}^{+\infty} \frac{\varphi(\xi, t)}{\sqrt{4\pi D(t-\tau)}} \exp\left(-\frac{(x-\xi)^2}{4D(t-\tau)}\right) d\xi d\tau. \quad (16)$$

Denoting by x_0 the characteristic width of the function $\varphi(x)$ and by $t_D = x_0^2/D$ the corresponding diffusion time, one can replace φ by the delta function if the inequalities $t_D \ll t \ll t_0$ are fulfilled and arrive, after integrating with respect to the coordinate, at an even simpler expression.

Consequently, the introduction of a delay time t_0 into the initial lifetime distribution brings about a deviation from the standard picture on the interval $\langle\tau\rangle < t < t_0$ even for the parameters β and γ corresponding to the conventional diffusion. The particles in the initial distribution decrease in number, according to Eq. (14), and serve as a source for the formation of the self-similar n_2 profile (16). This is so because of the absence of any internal scale in a power function. For instance, the exponential law is characterized by the time $\langle\tau\rangle$, which indicates that the function at $t = t_0 + \langle\tau\rangle$ decreases by e times compared to its value at $t = t_0$, irrespective of the chosen t_0. One can easily verify that such is not the case for a power function. Moreover, as t_0 increases, one is forced to wait an even longer time $t_1 \sim t_0$, after which the function decreases, e.g., twofold, and $t_1 \longrightarrow \infty$ for $t_0 \longrightarrow \infty$.

Let us now turn to the property (1). This problem differs from the preceding one in that the initial distribution N_0 is now not arbitrary but arises from the preliminary evolution of $\delta_+(\tau)$ during time t_1 according to Eqs. (3) and (4). In the case where the transport process is described asymptotically by the conventional diffusion equation, the time it takes for establishing the self-similar solution is determined by the microscopic time $\langle\tau\rangle$; i.e., Eq. (1) is fulfilled even at $t_1, t_2 \gg \langle\tau\rangle$. This is not the case for the subdiffusion regime. Let us apply the Laplace transform with respect to variables t_1 and t_2 to Eq. (1) and use the property

$$[f(t_1 + t_2)]_{p_1, p_2} = \frac{[f(t_1)]_{p_1} - [f(t_2)]_{p_2}}{p_2 - p_1}.$$

Then the relationship

$$\frac{G_{p_1} - G_{p_2}}{p_2 - p_1} = G_{p_2} G_{p_1}$$

must be fulfilled. One can easily verify that it is valid for the Green's function of the form (7) only if $p_2 \ll p_1$ or $t_2 \gg t_1$. This signifies that, depending on the duration t_1 of the first evolution stage, the time $t_2 \sim t_1$ is required for establishing the previous self-similar solution. The real transport process at times $t_2 \ll t_1$ can be described using the equations with a source on the right-hand side, as was done for the model problem with time delay (see above). However, in contrast to the example considered, a decrease in n_1 in this case and, correspondingly, an increase in the number of particles n_2 would be more rapid (at small t), because $N_0(\tau)$ is no longer concentrated at the far boundary $\tau = t_1$ but is extended over the entire interval $(0, t_1)$. For example, the source $q(x, t)$ in the equation for n_2 (cf. [12])

$$\frac{\partial^\gamma n_2(x, t)}{\partial t^\gamma} = \frac{1}{2}\frac{\partial^2 n_2}{\partial x^2} + q(x, t)$$

brings about an increase in n_2 according to the law

$$\int_{-\infty}^{+\infty} n_2(x, t) dx \propto t^{1-\gamma}.$$

In summary, we have demonstrated that the microscopic features of the initial distribution have a sizable effect on the process of stochastic transport. These features should be explicitly taken into account in the transport equation because they are responsible for the memory effects, specifically, for the dependence of the form of the equation on the macroscopic time. This additional degree of freedom allows the first stage of system evolution to be modified. This stage can be rather prolonged, as we have demonstrated by a model example where the effective equations are different from the classical diffusion equation even for the diffusional parameters of the problem (for the functions of class (2)). The number of particles in the initial condition linearly decreases with time to form a profile whose evolution is described by the diffusion equation with a constant source. The reason is that a power function describing the waiting time at any point for a particle executing random walk has no internal scale. Taking account of the initial distribution allows one to remove the main drawback consisting in the violation of evolution continuity in the asymptotic equation and use the subdiffusion equation with a time-independent source for the description of the transient process of profile formation by the particles of the initial distribution. We can say that the zero moment of a distribution function, i.e., the total number of particles, is insufficient for a correct description of the process. This function must be represented as a sum of terms, each corresponding to its own type of particles. A simple illustration of this approach is provided by the initial lifetime distribution in the form of a comb of shifted delta functions. However, it turns out that the division of particles even into two classes and the inclusion of the next moment of the distribution function (transition time from one sort of particles to the other) appreciably improves the accuracy of equations.

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