.

Generalized Master Equation with Two Times: Diffusion in External Field

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The generalized master equation with two times, introduced in [1,2], applies to the problem of diffusion in an time-dependent (in general inhomogeneous) external field. We consider the case of the quasi Fokker-Planck approximation, when the probability transition function for diffusion (PTD-function) does not possess a long tail in coordinate space and can be expanded as the function of instantaneous displacements. The more complicated case of the long tails in PTD will be discussed separately.

I. INTRODUCTION

The models of continuous time random walks (CTRW) [3], when some objects can jump from one point to another in inhomogeneous (in general) media and stay during some time in these points before the next usually stochastic jump, are important for the solution of many physical, chemical and biological problems. Recently these models have been applied also in economics and social sciences (see, e.g., [4-6]). Usually the stochastic motion of the particles leads to a second moment of the density distribution that is linear in time $< r^2(t) >\sim t$. Such type of the diffusion processes play a crucial role in plasmas, including dusty plasma [7], nuclear physics [8], neutral systems in various phases [9] and in many other problems. However, in many systems the deviation from the linear in time dependence of the mean square displacement have been experimentally observed, in particular, under essentially non-equilibrium conditions or for some disordered systems. The average square separation of a pair of particles passively moving in a turbulent flow grows, according to Richardson's law, with the third power of time [10]. For diffusion typical for glasses and related complex systems [11] the observed time dependence is slower than linear. These two types of anomalous diffusion obviously are characterized as superdiffusion and subdiffusion.

The generalized master equation for the density evolution, which describes the various cases of normal and anomalous diffusion has been formulated in [1,2] by introduction of the specific kernel function (PTD) depending on two times $W(\mathbf{r}, \mathbf{r}', \tau, t-\tau)$, which connects in a linear way the density distributions of the stochastic objects (or particles) f for the points $\mathbf{r}'$ at moment τ and $\mathbf{r}$ at moment t. The approach suggested in [1,2] clearly demonstrates the relation between the integral approach and the fractional differentiation method [12] and permits to extend (in comparison with the fractional differentiation method) the class of sub- and superdiffusion processes, which can be successfuly described. On this basis in [2] the different examples of superdiffusive and subdiffusive processes were considered for the various kernels W and the mean-squared displacements have been calculated. Recently the idea of the generalized master equation with two times [1,2] for diffusion in coordinate space has been recently used in [13] for the calculation of average displacements in the case of a time-dependent homogeneous external field.

This paper is motivated by the necessity to describe in more detail the influence of time- and space dependent external fields on the continuous-time random walks. The equation formulated in [1,2] is appropriate for this purpose and offers the opportunity for consideration of CTRW for both cases: long-tail space behavior of the PTD function, as well as for the fast decay of PTD function in coordinate space, when the Fokker-Planck type expansion is applicable. For simplicity in this paper we consider only the last case.

II. GENERALIZED MASTER EQUATION

Let us start from the generalized master equation with two times [1,2]:

$$f(\mathbf{r}, t) = f(\mathbf{r}, t=0) + \int_0^t d\tau \int d\mathbf{r}' \left\{ W(\mathbf{r}, \mathbf{r}', \tau, t-\tau) f(\mathbf{r}', \tau) - W(\mathbf{r}', \mathbf{r}, \tau, t-\tau) f(\mathbf{r}, \tau) \right\}. \quad (1)$$

Equation (1) can be represented in an equivalent form, more similar to the structure of the Fokker-Planck equation, where the initial condition is absent:

$$\frac{\partial f(\mathbf{r}, t)}{\partial t} = \frac{d}{dt} \int_0^t d\tau \int d\mathbf{r}' \left\{ W(\mathbf{r}, \mathbf{r}', \tau, t-\tau) f(\mathbf{r}', \tau) - W(\mathbf{r}', \mathbf{r}, \tau, t-\tau) f(\mathbf{r}, \tau) \right\}. \quad (2)$$

or

$$\frac{\partial f(\mathbf{r},t)}{\partial t} = \int_0^t d\tau \int d\mathbf{r}' \left\{ P(\mathbf{r},\mathbf{r}',\tau,t-\tau) f(\mathbf{r}',\tau) - P(\mathbf{r}',\mathbf{r},\tau,t-\tau) f(\mathbf{r},\tau) \right\}, \tag{3}$$

where the function $P(\mathbf{r},\mathbf{r}',\tau,t-\tau)$ is given by:

$$P(\mathbf{r},\mathbf{r}',\tau,t-\tau) \equiv 2W(\mathbf{r}',\mathbf{r},\tau,t-\tau)\delta(t-\tau) + \frac{\partial}{\partial t} W(\mathbf{r}',\mathbf{r},\tau,t-\tau) \tag{4}$$

The argument $t-\tau$ describes the retardation effects, which can be connected in the particular case of multiplicative PTD function $W(\mathbf{r},\mathbf{r}',\tau,t-\tau) \equiv W(\mathbf{r},\mathbf{r}',\tau)\chi(t-\tau)$ with, for example, the probability for the particles to stay during some time at the fixed coordinate before transition to the next point. An equation with retardation, where W function depends only on one time argument $t-\tau$ has been suggested first in [14] and applied in [15] to the case of the multiplicative representation of the PTD function. In general W is not a multiplicative function in the sense mentioned above and, what is more important, is a function of two times t and $t-\tau$ [1]. It is necessary to mention that the closed form of the equation for the density distribution is an approximation. In some cases the exact solution for density distribution can be found (see e.g. [16],[17]), when the closed equation for density distribution does not exist or gives an approximate result. Nevertheless, in many practical situations Eq. (1) or (4) are sufficiently exact and permit to describe various experimental data.

Let us consider the nature of appearance of the two time arguments in the generalized master equation Eq. (1) in the case of a time-dependent external force $\mathbf{F}(\mathbf{r},t)$. To simplify the consideration we can investigate the case of fast decay of the kernel $W(\mathbf{r},\mathbf{r}',\tau,t-\tau) \equiv W(\mathbf{u},\mathbf{r},\tau,t-\tau)$ as a function of $\mathbf{u} = \mathbf{r} - \mathbf{r}'$, when an expansion in the spirit of Fokker-Planck can be applied. In this case Eq. (1) takes the form [1,2]:

$$f(\mathbf{r},t) = f(\mathbf{r},t=0) + \int_0^t d\tau \frac{\partial}{\partial r_\alpha} \left[A_\alpha(\mathbf{r},\tau,t-\tau) f(\mathbf{r},\tau) + \frac{\partial}{\partial r_\beta} \left(B_{\alpha\beta}(\mathbf{r},\tau,t-\tau) f(\mathbf{r},\tau) \right) \right], \tag{5}$$

where the functions $A_\alpha(\mathbf{r},\tau,t-\tau)$ and $B_{\alpha\beta}(\mathbf{r},\tau,t-\tau) f_g(\mathbf{r},\tau)$ are the functionals of the PTD function (the indexes are equal $\alpha,\beta = x_s$ in s-dimensional coordinate space):

$$A_\alpha(\mathbf{r},\tau,t-\tau) = \int d^s u u_\alpha W(\mathbf{u},\mathbf{r},\tau,t-\tau) \tag{6}$$

and

$$B_{\alpha\beta}(\mathbf{r},\tau,t-\tau) = \frac{1}{2} \int d^s u\, u_\alpha u_\beta W(\mathbf{u},\mathbf{r},\tau,t-\tau). \tag{7}$$

Eq. (5) can be rewritten naturally in the form, corresponding to Eq. (2), but now for the Fokker-Planck type approximation:

$$\frac{\partial f(\mathbf{r},t)}{\partial t} = \frac{d}{dt}\int_0^t d\tau \frac{\partial}{\partial r_\alpha}\left[A_\alpha(\mathbf{r},\tau,t-\tau)f(\mathbf{r},\tau) + \frac{\partial}{\partial r_\beta}\left(B_{\alpha\beta}(\mathbf{r},\tau,t-\tau)f(\mathbf{r},\tau)\right)\right], \tag{8}$$

We suggest, that the PTD function is independent of $f(\mathbf{r},t)$, therefore the problem is linear.

III. INFLUENCE OF THE EXTERNAL FIELDS

One of the main sources of inhomogeneity is an external field, which also provides the prescribed dependence of the PTD function on τ. Other wards we can suggest, in the considered particular case, that the dependence of $W(\mathbf{u},\mathbf{r},\tau,t-\tau)$ on the arguments $\mathbf{r},\tau$ is connected with a functional dependence on an external field:

$$W(\mathbf{u},\mathbf{r},\tau,t-\tau) = W(\mathbf{u},t-\tau;\mathbf{F}(\mathbf{r},\tau)). \tag{9}$$

If the external fields are absent the PTD function is a function of the modulus $\mathbf{u} \equiv u$, which means that $A_\alpha = 0$ and $B = \delta_{\alpha\beta}B_0(t-\tau)$ with:

$$B_0(t-\tau) = \frac{1}{2s}\int d^s u\, u^2 W_0(u,t-\tau). \tag{10}$$

For relatively weak external fields the functional (9) can be linearized in the external field

$$W(\mathbf{u},t-\tau;\mathbf{F}(\mathbf{r},\tau)) = W_0(u,t-\tau) + W_1(u,t-\tau)(\mathbf{u}\cdot\mathbf{F}(\mathbf{r},\tau)). \tag{11}$$

The functions $W_0(u,t-\tau)$ and $W_1(u,t-\tau)$ are equal to $W(\mathbf{u},t-\tau;\mathbf{F}=0)$ and the functional derivative $\delta W(\mathbf{u},t-\tau;\mathbf{F}(\mathbf{r},\tau))/\delta(\mathbf{u}\cdot\mathbf{F}(\mathbf{r},\tau))_{|\mathbf{F}=0}$ respectively. Then the functions A_α and $B_{\alpha\beta}$ take the form

$$A_\alpha(\mathbf{r},\tau,t-\tau) = \frac{1}{s}\mathbf{F}_\alpha(\mathbf{r},\tau)\int d^s u u^2 W_1(u,t-\tau) \equiv \mathbf{F}_\alpha(\mathbf{r},\tau)L(t-\tau), \tag{12}$$

where $L(t-\tau)$ is given by

$$L(t-\tau) = \frac{1}{s}\int d^s u u^2 W_1(u,t-\tau). \tag{13}$$

and

$$B_{\alpha\beta}(\mathbf{r},\tau,t-\tau) = \delta_{\alpha\beta}B_0(t-\tau). \tag{14}$$

The generalized diffusion equation Eq. (8) takes the form

$$\frac{\partial f(\mathbf{r},t)}{\partial t} = \frac{d}{dt}\int_0^t d\tau \left[L(t-\tau)\nabla(\mathbf{F}(\mathbf{r},\tau)f(\mathbf{r},\tau)) + B_0(t-\tau)\Delta f(\mathbf{r},\tau)\right], \tag{15}$$

In general this equation contains two different functions B_0 and L depending on the argument $t-\tau$. If the functional $W(\mathbf{u}, t-\tau; \mathbf{F}(\mathbf{r},\tau))$ is multiplicative, namely, $W(\mathbf{u}, t-\tau; \mathbf{F}(\mathbf{r},\tau)) = \tilde{W}(\mathbf{u}; \mathbf{F}(\mathbf{r},\tau))\chi(t-\tau)$ Eq. (15) can be simplified:

$$\frac{\partial f(\mathbf{r},t)}{\partial t} = \frac{d}{dt}\int_0^t d\tau \chi(t-\tau)\left[D\Delta f(\mathbf{r},\tau) - b\nabla(\mathbf{F}(\mathbf{r},\tau)f(\mathbf{r},\tau))\right], \tag{16}$$

Here b and D are the constants, determined by the relations:

$$b = -\frac{1}{s}\int d^s u u^2 \tilde{W}_1(u) \tag{17}$$

with $\tilde{W}_1(u) = \delta\tilde{W}(\mathbf{u}; \mathbf{F}(\mathbf{r},\tau))/\delta(\mathbf{u}\cdot\mathbf{F}(\mathbf{r},\tau))_{|\mathbf{F}=0}$ and

$$D = \frac{1}{2s}\int d^s u u^2 \tilde{W}_0(u). \tag{18}$$

The physical sense of the multiplicative structure of the functional W is that independence of the time delay of the random walkers is independent of the external field. The dimensionless function $\chi(t)$ in this simple case is connected with the hopping-distribution function $\psi(t) = \lambda\psi^*(\lambda t)$ introduced in the master equation by Scher and Montroll [15]. The value $\lambda \equiv 1/\tau_0$ is the characteristic waiting time for the hopping-distribution. Laplace transformations of these functions $\chi(z)$ and $\psi^*(z)$ relate them as follows

$$\chi(z) = \frac{\psi^*(z)}{1-\psi^*(z)}. \tag{19}$$

For the exponential hopping-time distribution $\psi(t) = \lambda exp(-\lambda t)$, where $\lambda \equiv 1/\tau_0$ (τ_0 is the characteristic waiting time) we have $\psi^*(z) = 1/(1+z)$, $\chi(z) = 1/z$ and $\chi(t) \equiv \chi(\lambda t) = 1$. In this case Eq. (16) is reduced to the usual diffusion equation in an external field with the diffusion coefficient D and mobility b:

$$\frac{\partial f(\mathbf{r},t)}{\partial t} = D\Delta f(\mathbf{r},t) - b\nabla\left(\mathbf{F}(\mathbf{r},t)f(\mathbf{r},t)\right). \tag{20}$$

IV. CONCLUSIONS

We show that the generalized master equation with two times, which have been introduced in [1,2] can describe the influence of inhomogeneous and time-dependent external fields on the diffusion processes. Linearization of the general master equation in the external field leads to essential simplifications. In this case the diffusion processes depend, in general, on two different functions of time, which describe retardation due to the finite time of occupation and transferring particles in space in the presence of the external field. Relations with simpler models are established. The consideration in the present paper give the opportunity to consider a wide class of the problems of normal and anomalous transport in external fields on the basis of generalized master equations with two times.

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[1] S.A. Trigger, G.J.F. van Heijst, P.P.J.M. Schram, *Physica A*, 347, 77 (2005); http://arXiv.org/abs/physics/0401327

[2] S.A. Trigger, G.J.F. van Heijst, P.P.J.M. Schram, *J.of Physics: Confrence Series*, 11, 37 (2005)

[3] E.W. Montroll and M.F. Schlezinger in Studies in Statistical Mechanics, edited by J. Leibowitz and E.W. Montroll, V. 2 (North-Holland, Amsterdam, 1984)

[4] R. Mantegna, H. Stanley, Nature 376, 46 (1995)

[5] P. Gopikrishnan, V. Plerou, L. A. N. Amaral, M. Meyer, H.E. Stanley, *Phys. Rev.* E60, 5305 (1999).

[6] M. Newman, Contemporary Physics 46, 323 (2005)

[7] P.K. Schukla, A.A. Mamun, Introduction to Dusty Plasma Physics, Institute of Physics Publishing, Bristol, 2002.

[8] W.H. Stacey, Nuclear reactor physics, Wiley Publishing, 2001.

[9] Lecture Notes in Physics, LNP 557, Stochastic Processes in Physics, Chemistry and Biology, Edited by J.A. Freund and T. Poschel, Springer, 2002.

[10] A.S. Monin and A.M. Yaglom, Statistical Fluid Mechanics: Mechanics of Turbulence (MIT Press, Cambridge, MA, 1975), Vol II.

[11] B. Rinn, P. Mass, and J.P. Bouchaud, *Phys. Rev. Lett.* 84, 5405 (2000).

[12] B.J. West, M. Bologna, and P. Grigolini, *Physics of Fractal Operators*, (Springer-Verlag New York), 2003.

[13] I.M. Sokolov, *Phys. Rev.* E73, 067102 (2006), I.M. Sokolov and J. Klafter, arXiv: cond-mat/0606556, June 2006. In the one dimensional case, for a fixed length of a jump and a time-dependent homogeneous in space external field $\mathbf{F}(\tau)$ the authors obtained the diffusion equation with two times, which is a particular case of Eq.(73) [1] (see also Eq. (1), (2) of this paper). The particular result, using in [13], is similar to one-dimensional form of Eq. (16), which follows straightforward from the general equations of the papers [1],[2]. The authors overlooked the results of these papers. At the same time, as is necessary to mention, for the multiplicative kernel the force is placed under the integral over τ as it is in Eq. (16). Considering the more general Eq. (15) in the particular case, when $L(t-\tau)$ equals constant, we establish, that the term with an external field does not include the memory kernel and is proportional to usual mobility.

[14] V.M. Kenkre, E. Montroll and M.F. Schlezinger, *J. Stat. Phys.* 9, 45 (1973)

[15] H. Scher and E. Montroll, *Phys. Rev.* B12, 2455 (1975)

[16] C. Tsallis, D.J. Bukman, *Phys. Rev.* E54, R2197 (1996)

[17] V.Yu. Zaburdaev, Journal of Statistical Physics, accepted, in print, 2006 (private communications).