Generalized Transport Equation with Fractality of Space-Time. Zubarev's NSO Method

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Abstract: **We presented a general approach for obtaining the generalized transport equations with fractional derivatives by using the Liouville equation with fractional derivatives for a system of classical particles and the Zubarev nonequilibrium statistical operator (NSO) method within Renyi statistics. Generalized Cattaneo-type diffusion equations with taking into account fractality of space-time are obtained.**

Keywords: **fractional derivative, diffusion equation.**

I. Introduction

The fractional derivatives and integrals [1]–[4] are widely used to study anomalous diffusion in porous media, in disordered systems, in plasma physics, in turbulent, kinetic, and reaction-diffusion processes, etc. [5], [6]. In Ref. [5], [6], we discussed various approaches to obtaining the transport equations with fractional derivatives. It is important to note that, for the first time, in Refs. [7]–[10], Nigmatullin received diffusion equation with the fractional time derivatives for the mean spin density [7], the mean polarization [8], and the charge carrier concentration [9]. In Ref. [10], justification of equations with fractional derivatives is given, and the time irreversible Liouville equation with the fractional time derivative is provided. In our recent work [5], by using NSO method [11], [12] and the maximum entropy principle for the Renyi entropy, we obtained the generalized (non-Markovian) diffusion equation with fractional derivatives. The use of the Liouville equation with fractional derivatives proposed by Tarasov in Refs. [13], [14] is an important and fundamental step for obtaining this equation. By using NSO method and the maximum entropy principle for the Renyi entropy, we found a solution of the Liouville equation with fractional derivatives at a selected set of observed variables. We chose nonequilibrium average values of particle density as a parameter of reduced description, and then we received the generalized (non-Markovian) diffusion equation with fractional derivatives. In the next section by using Ref. [5], new non-Markovian diffusion equations for particles in a spatially heterogeneous environment with fractal structure are obtained. Different models of frequency-dependent memory functions are considered, and the diffusion equations with fractality of space-time are obtained.

II. Liouville Equation with Fractional Derivatives for System of Classical Particles

We use the Liouville equation with fractional derivatives obtained by Tarasov in Refs. [14] for a nonequilibrium particle function $\rho(x^N;t)$ of a classical system

$$\frac{\partial}{\partial t}\rho(x^N;t)+\sum_{j=1}^{N}D^{\alpha}_{\vec{r}_j}\Big(\rho(x^N;t)\vec{v}_j\Big)+\sum_{j=1}^{N}D^{\alpha}_{\vec{p}_j}\Big(\rho(x^N;t)\vec{F}_j\Big)=0, \quad (1)$$

where $x^N=x_1,\ldots,x_N$, $x_j=\{\vec{r}_j,\vec{p}_j\}$ are dimensionless generalized coordinates, $\vec{r}_j=(r_{j1},\ldots,r_{jm})$, and generalized momentum, $\vec{p}_j=(p_{j1},\ldots,p_{jm})$, [14] of j th particle in the phase space with a fractional differential volume element [13], [15] $d^{\alpha}V=d^{\alpha}x_1\ldots d^{\alpha}x_N$. Here, $m=Mr_0/(p_0t_0)$, M is the mass of particle, r_0 is a characteristic scale in the configuration space, p_0 is a characteristic momentum, and t_0 is a characteristic time, d^{α} is a fractional differential [15],

$$d^{\alpha}f(x)=\sum_{j=1}^{2N}D^{\alpha}_{x_j}f(x)(dx_j)^{\alpha},$$

where

$$D^{\alpha}_{x}f(x)=\frac{1}{\Gamma(n-\alpha)}\int_0^x\frac{f^{(n)}(z)}{(x-z)^{\alpha+1-n}}dz \quad (2)$$

is the Caputo fractional derivative, [1], [2], [16], [17] $n-1<\alpha<n$, $f^{(n)}(z)=d^nf(z)/dz^n$ with the properties $D^{\alpha}_{x_j}1=0$ and $D^{\alpha}_{x_j}x_l=0$, $(j\neq l)$. $\vec{v}_j$ are the fields of velocity, $\vec{F}_j$ is the force field acting on j th particle. If $\vec{F}_j$ does not depend on $\vec{p}_j$, $\vec{v}_j$ does not depend on $\vec{r}_j$, and the Helmholtz conditions, we get the Liouville equation in the form

$$\frac{\partial}{\partial t}\rho(x^N;t)+iL_{\alpha}\rho(x^N;t)=0, \quad (3)$$

where iL_{α} is the Liouville operator with the fractional derivatives,

$$iL_{\alpha}\rho(x^N;t)=\sum_{j=1}^{N}\Big[D^{\alpha}_{\vec{p}_j}H(\vec{r},\vec{p})D^{\alpha}_{\vec{r}_j}-D^{\alpha}_{\vec{r}_j}H(\vec{r},\vec{p})D^{\alpha}_{\vec{p}_j}\Big]\rho(x^N;t). \quad (4)$$

where $H(\vec{r},\vec{p})$ is a Hamiltonian of a system with fractional derivatives [13]. A solution of the Liouville equation (3) will be found with Zubarev's NSO method [11]. After choosing parameters of the reduced description, taking into account projections we present the nonequilibrium particle function $\rho(x^N;t)$ (as a solution of the Liouville equation) in the general form

$$\rho(x^N;t)=\rho_{rel}(x^N;t)-\int_{-\infty}^{t}e^{\varepsilon(t'-t)}T(t,t')(1-P_{rel}(t'))iL_{\alpha}\rho_{rel}(x^N;t')dt', \quad (5)$$

where $T(t,t') = \exp_+\left[-\int_{t'}^{t}(1-P_{rel}(t'))iL_\alpha dt'\right]$ is the evolution operator in time containing the projection, $\exp_+$ is ordered exponential, $\varepsilon \to +0$ after taking the thermodynamic limit, $P_{rel}(t')$ is the generalized Kawasaki-Gunton projection operator depended on a structure of the relevant statistical operator (distribution function), $\rho_{rel}(x^N;t')$. By using Zubarev's NSO method [11], [12] and approach, $\rho_{rel}\left(x^N;t'\right)$ will be found from the extremum of the Renyi entropy at fixed values of observed values $\langle\hat{P}_n(x)\rangle_\alpha^t$, taking into account the normalization condition $\langle 1\rangle_{\alpha,rel}^t = 1$, where the nonequilibrium average values are found respectively [5],

$$\langle\hat{P}_n(x)\rangle_\alpha^t = \hat{I}^\alpha(1,\ldots,N)\hat{T}(1,\ldots,N)\hat{P}_n\rho(x^N;t). \quad (6)$$

$\hat{I}^\alpha(1,\ldots,N)$ has the following form for a system of N particles $\hat{I}^\alpha(1,\ldots,N) = \hat{I}^\alpha(1),\ldots,\hat{I}^\alpha(N)$, $\hat{I}^\alpha(j) = \hat{I}^\alpha(\vec{r}_j)\hat{I}^\alpha(\vec{p}_j)$ and defines operation of integration

$$\hat{I}^\alpha(x)f(x) = \int_{-\infty}^{\infty} f(x)d\mu_\alpha(x), \quad d\mu_\alpha(x) = \frac{|x|^\alpha}{\Gamma(\alpha)}dx. \quad (7)$$

The operator $\hat{T}(1,\ldots,N) = \hat{T}(1),\ldots,\hat{T}(N)$ defines the operation $\hat{T}(x_j)f(x_j) = \frac{1}{2}(f(\ldots,x'_j - x_j,\ldots) + f(\ldots,x'_j + x_j,\ldots))$. Accordingly, the average value, which is calculated with the relevant distribution function, is defined as

$$\langle(\ldots)\rangle_{\alpha,rel}^t = \hat{I}^\alpha(1,\ldots,N)\hat{T}(1,\ldots,N)(\ldots)\rho_{rel}(x^N;t).$$

According to Ref. [12], from the extremum of the Renyi entropy functional

$$L_R(\rho') = \frac{1}{1-q}\ln\hat{I}^\alpha(1,\ldots,N)\hat{T}(1,\ldots,N)(\rho'(t))^q$$
$$-\gamma\hat{I}^\alpha(1,\ldots,N)\hat{T}(1,\ldots,N)\rho'(t)$$
$$-\sum_n\int d\mu_\alpha(x)F_n(x;t)\hat{I}^\alpha(1,\ldots,N)\hat{T}(1,\ldots,N)\hat{P}_n(x)\rho'(t)$$

at fixed values of observed values $\langle\hat{P}_n(x)\rangle_\alpha^t$ and the condition of normalization $\hat{I}^\alpha(1,\ldots,N)\hat{T}(1,\ldots,N)\rho'(t) = 1$, the relevant distribution function takes the form

$$\rho_{rel}(t) = \frac{1}{Z_R(t)}\left[1 - \frac{q-1}{q}\beta\left(H - \sum_n\int d\mu_\alpha(x)F_n(x;t)\delta\hat{P}_n(x;t)\right)\right]^{\frac{1}{q-1}}, \quad (8)$$

where $Z_R(t)$ is the partition function of the Renyi distribution, which is determined from the normalization condition and has the form

$$Z_R(t) = \hat{I}^\alpha(1,\ldots,N)\hat{T}(1,\ldots,N)$$
$$\times\left[1 - \frac{q-1}{q}\beta\left(H - \sum_n\int d\mu_\alpha(x)F_n(x;t)\delta\hat{P}_n(x;t)\right)\right]^{\frac{1}{q-1}}. \quad (9)$$

The Lagrangian multiplier γ is determined by the normalization condition. The parameters $F_n(x;t)$ are determined from the self-consistency conditions

$$\langle\hat{P}_n(x)\rangle_\alpha^t = \langle\hat{P}_n(x)\rangle_{\alpha,rel}^t. \quad (10)$$

It is important to note that the relevant distribution function corresponded to the Gibbs entropy follows from (8) at $q = 1$ [5]. In the general case of the parameters $\langle\hat{P}_n(x)\rangle_\alpha^t$ of the reduced description of nonequilibrium processes according to (5) and (8), we get NSO in the form

$$\rho(t) = \rho_{rel}(t)$$
$$+\sum_n\int d\mu_\alpha(x)\int_{-\infty}^{t} e^{\varepsilon(t'-t)}T(t,t')I_n(x;t')\rho_{rel}(t')\beta F_n^*(x;t')dt', \quad (11)$$

where $F_n^*(x;t') = \dfrac{F_n(x;t')}{1 + \frac{q-1}{q}\sum_n\int d\mu_\alpha(x)F_n(x;t')\langle P_n(x)\rangle_\alpha^t}$,

$$I_n(x;t') = \left(1 - P(t)\right)\tfrac{1}{q}\psi^{-1}(t)iL_\alpha\hat{P}_n(x) \quad (12)$$

are the generalized flows, $P(t)$ is the Mori projection operator [5], and the function $\psi(t)$ has the following structure $\psi(t) = 1 - \frac{q-1}{q}\sum_n\int d\mu_\alpha(x)F_n(x;t)P_n(x)$.

By using the nonequilibrium statistical operator (11), we get the generalized transport equation for the parameters $\langle\hat{P}_n(x)\rangle_\alpha^t$ of the reduced description,

$$\frac{\partial}{\partial t}\langle\hat{P}_n(x)\rangle_\alpha^t = \langle iL_\alpha\hat{P}_n(x)\rangle_{\alpha,rel}^t$$
$$+\sum_{n'}\int d\mu_\alpha(x')\int_{-\infty}^{t} e^{\varepsilon(t'-t)}\varphi_{P_nP_{n'}}(x,x';t,t')\beta F_{n'}^*(x';t')dt', \quad (13)$$

where

$$\varphi_{P_nP_{n'}}(x,x';t,t') = \hat{I}^\alpha(1,\ldots,N)\hat{T}(1,\ldots,N)$$
$$\times\left(iL_\alpha\hat{P}_n(x)T(t,t')I_{n'}(x';t')\rho_{rel}(x^N;t')\right) \quad (14)$$

are the generalized transport kernels (the memory functions), which describe dissipative processes in the system. To demonstrate the structure of the transport equations (13) and the transport kernels (14), we will consider, for example, diffusion processes. In the next section, we obtain generalized transport equations with fractional derivatives and consider a concrete example of diffusion processes of the particle in non-homogeneous media.

III. Generalized Diffusion Equations with Fractional Derivatives

One of main parameters of the reduced description to describe the diffusion processes of the particles in non-homogeneous media with fractal structure is the nonequilibrium density of the particle numbers, $\langle\hat{P}_n(x)\rangle_\alpha^t$: $n(\vec{r};t) = \langle\hat{n}(\vec{r})\rangle_\alpha^t$, where $\hat{n}(\vec{r}) = \sum_{j=1}^{N}\delta(\vec{r} - \vec{r}_j)$ is the microscopic density of the particles. The corresponding generalized diffusion equation for $n(\vec{r};t)$ can be obtained on base of Eqs. (8), (11), (13),

$$\frac{\partial\langle\hat{n}(\vec{r})\rangle_\alpha^t}{\partial t} = \frac{\partial^\alpha}{\partial\vec{r}^\alpha}\cdot\int d\mu_\alpha(\vec{r}')\int_{-\infty}^{t} e^{\varepsilon(t'-t)}D_q(\vec{r},\vec{r}';t,t')\cdot\frac{\partial^\alpha\beta\nu^*(\vec{r}';t')}{\partial\vec{r}'^\alpha}dt', \quad (15)$$

where

$$D_q(\vec{r},\vec{r}';t,t') = \langle\hat{\vec{v}}(\vec{r})T(t,t')\hat{\vec{v}}(\vec{r}')\rangle_{\alpha,rel}^t \quad (16)$$

is the generalized coefficient diffusion of the particles within the Renyi statistics. Averaging in Eq. (16) is performed with the power-law Renyi distribution,

$$\rho_{rel}(t)=\frac{1}{Z_R(t)}\left(1-\frac{q-1}{q}\beta\left(H-\int d\mu_\alpha(\vec r)\nu^*(\vec r;t)\hat n(\vec r)\right)\right)^{\frac{1}{q-1}}, \quad (17)$$

where

$$Z_R(t)=\hat I^\alpha(1,\dots,N)\hat T(1,\dots,N)$$
$$\times\left(1-\frac{q-1}{q}\beta\left(H-\int d\mu_\alpha(\vec r)\nu^*(\vec r;t)\hat n(\vec r)\right)\right)^{\frac{1}{q-1}} \quad (18)$$

is the partition function of the relevant distribution function, H is a Hamiltonian of the system, q is the Renyi parameter ($0<q<1$).

Parameter $\nu(\vec r;t)$ is the chemical potential of the particles, which is determined from the self-consistency condition,

$$\langle\hat n(\vec r)\rangle_\alpha^t=\langle\hat n(\vec r)\rangle_{\alpha,rel}^t. \quad (19)$$

$\beta=1/k_\mathrm{B}T$ (k_B is the Boltzmann constant), T is the equilibrium value of temperature, $\hat{\vec v}(\vec r)=\sum_{j=1}^N\vec v_j\delta(\vec r-\vec r_j)$ is the microscopic flux density of the particles. At $q=1$, the generalized diffusion equation within the Renyi statistics goes into the generalized diffusion equation within the Gibbs statistics with fractional derivatives. If $q=1$ and $\alpha=1$, we obtain the generalized diffusion equation within the Gibbs statistics. In the Markov approximation, the generalized coefficient of diffusion in time and space has the form $D_q(\vec r,\vec r';t,t')\approx D_q\delta(t-t')\delta(\vec r-\vec r')$. And by excluding the parameter $\nu^*(\vec r';t')$ via the self-consistency condition, we obtain the diffusion equation with fractional derivatives from Eq. (15)

$$\frac{\partial}{\partial t}\langle\hat n(\vec r)\rangle_\alpha^t=\sum_b D_q\frac{\partial^{2\alpha}}{\partial r^{2\alpha}}\nu^*(\vec r';t'). \quad (20)$$

The generalized diffusion equation takes into account spatial fractality of the system and memory effects in the generalized coefficient of diffusion $D_q(\vec r,\vec r';t,t')$ within the Renyi statistics. Obviously, spatial fractality of system influences on transport processes of the particles that can show up as multifractal time with characteristic relaxation times. It is known that the nonequilibrium correlation functions $D_q(\vec r,\vec r';t,t')$ can not be exactly calculated, therefore the some approximations based on physical reasons are used. In the time interval $-\infty\div t$, ion transport processes in spatially non-homogeneous system can be characterized by a set of relaxation times that are associated with the nature of interaction between the particles and particles of media with fractal structure. To show the multifractal time in the generalized diffusion equation, we use the following approach for the generalized coefficient of particle diffusion

$$D_q(\vec r,\vec r';t,t')=W(t,t')\overline{D}_q(\vec r,\vec r'), \quad (21)$$

where $W(t,t')$ can be defined as the time memory function. In view of this, Eq. (15) can be represented as

$$\frac{\partial}{\partial t}\langle\hat n(\vec r)\rangle_\alpha^t=\int_{-\infty}^t e^{\varepsilon(t'-t)}W(t,t')\Psi(\vec r;t')dt', \quad (22)$$

where

$$\Psi(\vec r;t')=\int d\mu_\alpha(\vec r')\frac{\partial^\alpha}{\partial\vec r^\alpha}\cdot\overline{D}_q(\vec r,\vec r')\cdot\frac{\partial^\alpha}{\partial\vec r'^\alpha}\beta\nu^*(\vec r';t'). \quad (23)$$

Further we apply the Fourier transform to Eq. (22), and as a result we get in frequency representation

$$i\omega n(\vec r;\omega)=W(\omega)\Psi(\vec r;\omega). \quad (24)$$

We can represent the frequency dependence of the memory function in the following form

$$W(\omega)=\frac{(i\omega)^{1-\xi}}{1+i\omega\tau},\quad 0<\xi\le 1, \quad (25)$$

where the introduced relaxation time τ_a characterizes the particles transport processes in the system. Then Eq. (24) can be represented as

$$(1+i\omega\tau)i\omega n(\vec r;\omega)=(i\omega)^{1-\xi}\Psi(\vec r;\omega). \quad (26)$$

Further we use the Fourier transform to fractional derivatives of functions,

$$L\left({}_0D_t^{1-\xi}f(t);i\omega\right)=(i\omega)^{1-\xi}L(f(t);i\omega). \quad (27)$$

By using it, the inverse transformation of Eq. (26) to time representation gives the Cattaneo-type generalized diffusion equation with taking into account spatial fractality,

$$\tau\frac{\partial^2}{\partial t^2}n(\vec r;t)+\frac{\partial}{\partial t}n(\vec r;t)={}_0D_t^{1-\xi}\Psi(\vec r;t)=\frac{\partial^{1-\xi}}{\partial t^{1-\xi}}\Psi(\vec r;t), \quad (28)$$

which is the new Cattaneo-type generalized equation within the Renyi statistics with multifractal time and spatial fractality. At $q=1$ from Eq. (29), we get the Cattaneo-type generalized equation within the Gibbs statistics with multifractal time and spatial fractality,

$$\tau\frac{\partial^2}{\partial t^2}n(\vec r;t)+\frac{\partial}{\partial t}n(\vec r;t)={}_0D_t^{1-\xi}\int d\mu_\alpha(\vec r')\frac{\partial^\alpha}{\partial\vec r^\alpha}\cdot\overline{D}(\vec r,\vec r')\cdot\frac{\partial^\alpha}{\partial\vec r'^\alpha}\beta\nu(\vec r';t), \quad (29)$$

Eqs. (28), (29) contain significant spatial non-homogeneity in $\overline{D}_q(\vec r,\vec r')$. If we neglect spatial non-homogeneity,

$$\overline{D}_q(\vec r,\vec r')=\overline{D}_q\delta(\vec r-\vec r'), \quad (30)$$

we get the Cattaneo-type diffusion equation with fractality of space-time and the constant coefficients of the diffusion within the Renyi statistics,

$$\tau\frac{\partial^2}{\partial t^2}n(\vec r;t)+\frac{\partial}{\partial t}n(\vec r;t)={}_0D_t^{1-\xi}\overline{D}_q\frac{\partial^{2\alpha}}{\partial\vec r^{2\alpha}}\beta\nu^*(\vec r;t), \quad (31)$$

At $q=1$, we get the Cattaneo-type diffusion equation with fractality of space-time and the constant coefficients of the diffusion within the Gibbs statistics,

$$\tau\frac{\partial^2}{\partial t^2}n(\vec r;t)+\frac{\partial}{\partial t}n(\vec r;t)={}_0D_t^{1-\xi}\sum_b\overline{D}\frac{\partial^{2\alpha}}{\partial\vec r^{2\alpha}}\nu(\vec r;t), \quad (32)$$

It should be noted that if we put $\alpha=1$ in Eqs. (31), (32), i.e. we neglect spatial fractality, we get the Cattaneo-type diffusion equations, which were obtained in Ref. [18],

$$\tau\frac{\partial^2}{\partial t^2}n(\vec r;t)+\frac{\partial}{\partial t}n(\vec r;t)={}_0D_t^{1-\xi}\overline{D}\frac{\partial^2}{\partial\vec r^2}\nu(\vec r;t). \quad (33)$$

At $\tau = 0$, we get an important particular case — the generalized diffusion equation of particles with taking into account fractality of space-time,

$$\frac{\partial}{\partial t} n(\vec{r};t) = {}_0D_t^{1-\xi} \int d\mu_\alpha(\vec{r}') \frac{\partial^\alpha}{\partial \vec{r}^\alpha} \cdot \overline{D}_q(\vec{r},\vec{r}') \cdot \frac{\partial^\alpha}{\partial \vec{r}'^\alpha} \beta \nu^*(\vec{r}';t), \quad (34)$$

and by neglecting spatial non-homogeneity of the diffusion coefficients $\overline{D}_q(\vec{r},\vec{r}')$, we also get the diffusion equation with the constant coefficients of the diffusion with the fractional derivatives within the Renyi statistics,

$$\frac{\partial}{\partial t} n(\vec{r};t) = {}_0D_t^{1-\xi} \overline{D}_q \frac{\partial^{2\alpha}}{\partial \vec{r}^{2\alpha}} \beta \nu^*(\vec{r};t), \quad (35)$$

At $\alpha = 1$, $\tau = 0$, we get the diffusion equation with the constant coefficients of the diffusion without spatial fractality within the Renyi statistics

$$\frac{\partial}{\partial t} n(\vec{r};t) = {}_0D_t^{1-\xi} \overline{D}_q \frac{\partial^2}{\partial \vec{r}^2} \beta \nu^*(\vec{r};t), \quad (36)$$

At $\alpha = 1$, $\tau = 0$, $q = 1$, $\xi = 1$, we get the usual diffusion equation for the particles within the Gibbs statistics,

$$\frac{\partial}{\partial t} n(\vec{r};t) = \overline{D} \frac{\partial^2}{\partial \vec{r}^2} \beta \nu(\vec{r};t). \quad (37)$$

Let us consider another model of the memory function

$$W(\omega) = \frac{(i\omega)^{1-\xi}}{1 + (i\omega\tau)^{\gamma-1}}, \quad (38)$$

then in frequency representation we get

$$\left(1 + (i\omega\tau)^{\gamma-1}\right) i\omega n(\vec{r};\omega) = (i\omega)^{1-\xi} \Psi(\vec{r};\omega). \quad (39)$$

By using Eq. (27) and inverse transformation of Eq. (39) to the time t, we get the generalized Cattaneo-type diffusion equation with taking into account multifractal time and spatial fractality.

IV. CONCLUSION

We presented the general approach for obtaining the generalized transport equations with the fractional derivatives by using the Liouville equation with the fractional derivatives [14] for a system of classical particles and Zubarev's NSO method within the Renyi statistics [5]. In this approach, the new non-Markov equations of diffusion of the particles in a spatially non-homogeneous medium with a fractal structure are obtained.

By using approaches for the memory functions and fractional calculus [1]–[5], the generalized Cattaneo-type diffusion equations with taking into account fractality of space-time are obtained. It is considered the different models for the frequency dependent memory functions, which lead to the known diffusion equations with the fractality of space-time and their generalizations.

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