The Stochastical Model of Approximation of the Solution of Subdiffusion Equation

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Abstract -**The stochastical model of the dynamics equation of concentration of particles is used for constructing the approximation of the solution of the subdiffusion equation with fractional time derivative.**

I. INTRODUCTION

The purpose of this paper is to construct the algorithm of numerical realization of solution of the evolutionary equation of subdiffusion with fractional time derivative. The algorithm is found on the stochastical model realizing the density dynamics of particles.

It is known that the balance equations for the particles of medium, or the density dynamics equations, with special requirements to the stochastic distribution of random wandering gives the models of classical diffusion, subdiffusion or superdiffusion, [1], [2].

Evolutionary equations of subdiffusion and superdiffusion contain the fractional derivatives by time and space arguments correspondingly. One of derivations of these equations introdused in [1] is found on the spectral representation and treats the power behavior of the possibilities of "jumps" and "waitings" of particles. The power order of stochastic distribution determines the order of fractional derivative in the evolutionary equation.

Stochastic methods of approximation of the solutions of equations are well-known and in different modifications have being applied for numerical realization of transcalency equation, telegraph equation and so on (with integer derivatives), [7].

In this paper the method of approximation is developed for the solution of subdiffusion equation. It found on the invertion of the derivation scheme offered in [1]. The scheme of derivation of the evolutionary equation is on table 1:

TABLE I
THE SCHEME OF APPROXIMATION

I. The stochastic generation of particles

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II. Difference-integral equation of density of particles

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III. Spectral representation and tend to limit in spectral domain

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IV. The invertion of the transform (Laplas, Fourie), resulting with the evolutionary equation with fractional derivative

We build the invertion of this scheme stepwise. For evolutionary equation of subdiffusion with given order of fractional time derivative and given coeffitient the stochastic distribution is determined, which simulate the "memory" of particle in a fixed point of space. On the base of this generator the numerical approximation of integro-differential equation of the density dynamics is simulated. According to the scheme, the constructed numerical approximation of integro-differential equation is the solution of the original evolutionary equation with fractional time derivative.

II. THE TRANSFORMATION OF THE BALANCE EQUATION IN THE CASE OF FINIT CHARACTERISTICS

The modelling of transfer processes distinguishes two fundamentally different approaches. The first approach is classical, it takes place when the mean-square deviation, $<x^2>$, and the mean time of staying of particle in the point, $<t>$, are finit. The second case is called in actual literature the anomalous diffusion, [1]–[3], it deals with infinite values of these characteristics.

Let's specify in the beginning some details of a conclusion of the differential equation of the classical diffusion, based on limitation of characteristics $< x^2 >$ and $<t>$.

Given *f(t)* – the density of probability to make a jump in the adjacent points after time *t* being in the present point. Note that *f* is independent of the space position *x*. For *f(t)*

$$\int_0^\infty f(t)\,dt = 1; \qquad < t > = \int_0^\infty t \cdot f(t)\,dt. \tag{1}$$

Following [1] we choose

$$f(t) = \frac{a}{(1+t)^a}, \qquad 0 < a \le 1. \tag{2}$$

For our convenience denote the function *F (t)* – probability of particle being in a point *x* longer time than *t*.

$$F(t) = 1 - \int_0^t f(r)dr.$$

So we have

$$F(t) = \frac{1}{(1+t)^a}. \tag{3}$$

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Let *P(x,t,r)* be the density distribution of time *r* of particle being in the point. Then the density of points is given by

$$p(x,t) = \int_0^\infty P(x,t,r)\,dr$$

The equation of density dynamics of particles we take in the form, [1],

$$p(x,t)=\frac{1}{2}\int_0^t \left(p(x-1,t-r)+p(x+1,t-r)\right) f(r)\,dr + p_0(x)\cdot F(t) \qquad (4)$$

where $p_0(x)=p(x,0)$ is the starting density distribution.

In the case of $<t> \neq \infty$ and $<x^2> \neq \infty$ the integral equation of balance (4) transformes to the differential equation after the decomposing in Teilor series,

$$p(x,t)-\int_0^t p(x,t-r)f(r)\,dr = \frac{1}{2}\int_0^t (p(x-1,t-r)- -2p(x,t-r)+p(x+1,t-r))f(r)\,dr + p_0(x)\cdot F(t),$$

then

$$p(x,t)-p(x,t)\cdot\int_0^t f(r)\,dr+\frac{\partial p(x,t)}{\partial t}\cdot\int_0^t r\cdot f(r)\,dr = \frac{\Delta x^2}{2}\frac{\partial p^2(x,t)}{\partial x^2}+\frac{\Delta x^2}{2}\frac{\partial p^3(x,t)}{\partial t\partial x^2}\cdot\int_0^t r\cdot f(r)\,dr + p_0(x)\cdot F(t)+O(\Delta x^4)$$

that gives in limit the diffusion equation

$$\frac{\partial p(x,t)}{\partial t} = D\frac{\partial^2 p(x,t)}{\partial x^2}+p_0(x)\cdot\frac{F(t)}{<t>}, \qquad (5)$$

where D is the diffusion coefficient,

$$D=\frac{<x^2>}{2\cdot <t>}$$

Depending on the specialities of wandering at the microscopic scale the macroscopic transition equations may differ essentially from the classical diffusion equation.

When the stochastic distribution have the power behavior the power low of wandering appears

$$<x^2> \propto t^a.$$

In the case $a=\frac{1}{2}$ the classical diffusion takes place, else we have the anomalous diffusion.

When $a>\frac{1}{2}$ the process is *superdiffusion*. For this type of anomalous diffusion we can't ignore the very long runs of particles in medium because $<x^2> = \infty$.

In the case $a<\frac{1}{2}$ the process is *subdiffusion*. For this type of anomalous diffusion the very long time of waiting of the run from one point of space to another is possible, $<t> = \infty$. The subdiffusion process is modelled nowadays, [1], [2], by distributed in space traps with infinite mean time of particle waitings in it.

The particle may exist at one of the two states – at usual diffusion and at the rest (after falling into a trap). The subdiffusion process is the sequential change of these states in the random time moments. The medium is considered as the discrete set of points.

Note important thing for us: in a case when characteristics $<x^2>$ and $<t>$ are infinite, the reduction of the equation of balance (4) to the (5) is impossible. We will consider the case $<t> = \infty$ and being incapable of using decomposition in Teilor series we will apply our scheme, see Tab.1.

III. ABOUT THE SPECTRAL REPRESENTATION OF THE STOCHASTIC TRANSFERE PROCESS IN THE CASE OF SUBDIFFUSION

In te case $<t> = \infty$ we can rewrite the balance equation (4) as follows

$$p(x,t)-\int_0^t p(x,t-r)\cdot f(r)\,dr = \frac{1}{2}\int_0^t (p(x-1,t-r)+p(x+1,t-r)) -2p(x,t-r)f(r)\;dr+p_0(x)\cdot F(t). \qquad (6)$$

Consider representation of this expression in spectral area. We take its Laplas transform, [3], by time variable *t*.

Remind, that Laplas transformation of function *g(t)* is function

$$L(g(t)) = G(s) = \int_0^\infty e^{-st} g(t)\,dt.$$

Accordingly, the inverse Laplas transformation is defined as

$$\frac{1}{2\pi i}\int_{t-i\infty}^{t+i\infty} e^{st}G(s)\,ds = \begin{cases} g(t), & t\ge 0 \\ 0, & t<0 \end{cases}.$$

The Laplas transformation is continuous and it is one-to-one for continuous functions.

We denote the Laplas transformations of functions p(x,s), f(s) and F(s) by functions $p_s(x,s)$, $f_s(s)$ and $F_s(s)$ correspondingly.

Calculating the Laplas transformation from the left part of the equation (6) we obtain

$$L\left(p(x,t)-\int_0^t p(x,t-r)\cdot f(r)\,dr\right) =$$

$$= p_s(x,s) - p_s(x,s)\cdot f_s(s) = p_s(x,s)\cdot(1-f_s(s)) \quad (7)$$

Let's find $f_s(s)$.

$$f_s(s) = \int_0^\infty e^{-st}\frac{a}{(1+t)^{a+1}}dt = \\ = a\int_0^\infty \frac{e^{-(s+st)}\cdot e^s}{(s+st)^{a+1}\cdot s^{-a-1}\cdot s}d(st) = ,\\ = a\cdot e^s\cdot p^a\cdot\Gamma(-a,s)$$

where $\Gamma(-a,s)=\int_s^\infty e^{-r}r^{-a-1}\,dr$ is incomplete gamma-function. Similarly

$$F_s(s) = \int_0^\infty e^{-st}\frac{1}{(1+t)^a}dt = e^s\cdot p^{a-1}\cdot\Gamma(1-a,s) \; .$$

Accorging to (3)

$$F_s(s) = \int_0^\infty e^{-st}\left(1-\int_0^t f(r)\,dr\right)dt = \\ = \int_0^\infty e^{-st}\,dt - \frac{1}{s}\cdot f_s(s) = \frac{1}{s}(1-f_s(s))$$

Then the expression from (7) is equal to $p_s(x,s)\cdot sF_s(s)$. The Laplas transformation of the right part (6) is

$$\frac{1}{2}f_s(s)\big(p_s(x-1,s)-2p_s(x,s)-p_s(x+1,s)\big)+ \\ +p_0(x)\cdot F_s(s)$$

So, the Laplas transformation of the initial balance equation (4) is

$$p_s(x,s)\cdot sF_s(s) = \\ =\frac{1}{2}f_s(s)\big(p_s(x-1,s)-2p_s(x,s)-p_s(x+1,s)\big)+ \quad (8)\\ +p_0(x)\cdot F_s(s)$$

IV. CONVERSION IN THE SPECTRAL DOMAIN AND THE DERIVATION OF THE EVOLUTIONARY EQUATION OF SUBDIFFUSION

According to [1], we derive from (8) the evolutionary equation of subdiffusion with fractional time derivative.

Decomposing (8) in Teilor series, we receive

$$p_s(x,s)\cdot sF_s(s) = \\ =\frac{\Delta x^2}{2}f_s(s)\cdot\frac{\partial^2 p_s(x,s)}{\partial x^2}+p_0(x)\cdot F_s(s)+\mathrm{O}(\Delta x^4),$$

That is equivalent to, see (2)-(3),

$$e^s\cdot s^a\cdot\Gamma(1-a,s)\cdot p_s(x,s) = \\ =a\cdot e^s\cdot s^a\cdot\Gamma(-a,s)\cdot\frac{\Delta x^2}{2}\cdot\frac{\partial^2 p_s(x,s)}{\partial x^2} + \\ + e^s\cdot s^{a-1}\cdot\Gamma(1-a,s)\cdot p_0(x)+\mathrm{O}(\Delta x^4)$$

Multiply this equation on $e^{-s}\cdot\frac{\Gamma(1-a)}{\Gamma(1-a,s)}$. The first component in the right part will be transformed as

$$a\cdot s^a\cdot\Gamma(-a,s)\frac{\Gamma(1-a)}{\Gamma(1-a,s)}\cdot\frac{\Delta x^2}{2}\cdot\frac{\partial^2 p_s(x,s)}{\partial x^2}.$$

For incomplete gamma-function $\Gamma(b,s)$

$$\frac{\Gamma(b)}{\Gamma(b,s)}\to 1 \;\; with \;\; s\to 0$$

and

$$b\cdot\Gamma(b,s) = b\cdot\int_s^\infty e^{-r}r^{b-1}\,dr = \int_s^\infty e^{-r}\,d(r^b) = \\ =\Gamma(b+1,s)-e^{-s}\cdot s^b.$$

Then under conditions *s<<1* and *a<1*, (8) may be rewritten to a kind

$$s^a\cdot\Gamma(1-a)\cdot p_s(x,s) = \\ =s^a\cdot\Gamma(-a)\cdot\frac{\Delta x^2}{2}\cdot\frac{\partial^2 p_s(x,s)}{\partial x^2}+s^{a-1}\cdot\Gamma(1-a)\cdot p_0(x). \quad (9)$$

The inverse Laplas transformation of (9) gives the evolutionary equation in physical coordinates

$$\frac{\partial^a p(x,t)}{\partial t^a} = D_0\frac{\partial^2 p(x,t)}{\partial x^2}+p_0(x)\cdot\frac{F(t)}{t^a}. \quad (10)$$

Where D_0 is some coefficient.

This equation is called the subdiffusion equation corresponding to the memory distribution (2)–(3).

V. THE STOCHASTIC METHOD OF APPROXIMATION OF THE SOLUTION OF SUBDIFFUSION EQUATION

Note that the fractional order of differentiation on time in physical coordinates of the equation (10) corresponds exactly to a power coefficient in distribution (2). It allows us to introduce the algorithm of numerical realization of the solution of equation (10) in conditions

$$p(x,t)\Big|_{t=0} = p_0(x)\,, \qquad (11)$$

We model the distribution of particles to small time intervals $[0,\ t_1]$, $[t_1, t_2]$, ... $[t_{n-1}, t_n]$, where $t_{k+1} - t_k = \frac{t}{n}$. Accordingly to the integro-differential equation (4) we can write out

$$p(x,t_k) = \frac{1}{2}\int_{t_{k-1}}^{t_k} \left(p(x-\Delta x, t_k - r) + p(x+\Delta x,\ t_k r) \right) f(r)\,dr +$$

$$+\ p_0(x)\cdot F(t_k) \quad (12)$$

Where $k=1,\ldots, n,\ \ t_0 = 0\,,\ t_n = t\,.$

At $t_n = t$ we receive *p (x, t)* which, according to stages III-IV the Tab.1, is the decision of an initial equation (11) for the equation of subdiffusion (10).

V. CONCLUSION

The composition of models of the classical diffusion and the "traps" representing the memory of particles, distributed by law (2), satisfies integto-difference equation of dynamics of concentration (4). The equation (4) under an additional condition $< t > = \infty$ is equivalent to the equation (10) with the initial data (11). It allows us to realize the stochastic algorithm (12) of numerical approximation of the decision of an initial equation (10), (11).

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