HYPERBOLIC SUBDIFFUSION–REACTION EQUATION

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Subdiffusion occurs in a medium where the mobility of particles is strongly hindered due to the internal structure of the medium as, for example, in porous media or gels. The most commonly used differential equation described anomalous diffusion is the following equation with the Riemann–Liouville fractional derivative

$$\frac{\partial}{\partial t}P(x,t) = D_\alpha \frac{\partial^{1-\alpha}_{RL}}{\partial t^{1-\alpha}} \frac{\partial^2}{\partial x^2}P(x,t) \,, \tag{1}$$

the derivative is defined for $\alpha > 0$ as follows

$$\frac{d^\alpha_{RL}}{dt^\alpha}f(t) = \frac{1}{\Gamma(n-\alpha)}\frac{d^n}{dt^n}\int_0^t (t-t')^{n-\alpha-1}f(t')dt' \,, \tag{2}$$

n is a natural number fulfilled $\alpha \leq n < \alpha + 1$. Equation (1) was derived within the continuous time random walk formalism.

The fundamental solution to Eqs. (1) (the Green function), which is defined by its initial condition $P(x,t;x_0) = \delta(x-x_0)$ is interpreted as a probability density to find a random walker at point x after time t under the condition that its initial position is x_0. However, it is well known that the Green function of Eq. (1) has a non–physical property. Namely, it has non–zero values for any x at $t > 0$. This means that some of the particles moves with an arbitrarily chosen large velocity. To avoid this absurdity the persistent random walk model was proposed. Under the assumption that the actual random walker's step is correlated with the previous one, which means that the direction of successive steps is kept with probability β. For the normal diffusion process one obtains the following differential hyperbolic Cattaneo equation

$$\tau\frac{\partial^2}{\partial t^2}P(x,t) + \frac{\partial}{\partial t}P(x,t) = D\frac{\partial^2}{\partial x^2}P(x,t) \,, \tag{3}$$

where D is the normal diffusion coefficient, the parameter τ depends on β. A solution to this equation is above zero in a finite domain only, which ensures that a random walker's velocity is limited. We mention here that one of the simplest interpretations of this process is that the probability flux is delayed over time by parameter τ with respect to the probability gradient, $J(x,t+\tau) = -D\frac{\partial}{\partial x}P(x,t)$. Assuming $\tau \ll t$ there is $J(x,t) + \tau\frac{\partial}{\partial t}J(x,t) = -D\frac{\partial}{\partial x}P(x,t)$. Combining the above equation with the continuity equation $\frac{\partial}{\partial t}P(x,t) = -\frac{\partial}{\partial x}J(x,t)$, one obtains Eq. (3). For $\tau = 0$ we have the normal diffusion equation. The generalization of Eq. (3) to the subdiffusion system is not obvious. There are various forms of a such generalization, which are not equivalent to each other.

In this contribution a new hyperbolic subdiffusion–reaction equation was derived [1]. Starting with the difference equation, which describes a persistent random walk in a system with chemical reactions, using the generating function method and the continuous time random walk formalism, we will derive the hyperbolic–type subdiffusion differential equation with fractional time derivatives in which the chemical reactions $A + B(static) \rightarrow B(static)$ are taken into account. We will also find its solution over a long time limit. Based on the obtained results, we will find the hyperbolic–type subdiffusion–reaction equation in the case in which mobile particles of species A and B can chemically react according to a more complicated rule.

Persistent random walk is a process with memory, as well as subdiffusion. There arises a question: are these two effects simultaneously worth considering? The subdiffusive memory effect, controlled by the parameter α, is long and vanishes in the case of normal diffusion. The persistent random walk memory effect, which arises from the correlation of the successive random walker's steps, is relatively short. This is controlled by parameter β, which is assumed to be independent of α. We show that the parameter β significantly influences the solutions of subdiffuion–reaction equation. The considerations presented in this paper show that the effect of step correlations changes the effective subdiffusion parameter D_α and provides new terms in the subdiffusion–reaction equation which can change the dynamic of the process (at least in some situations). We will also briefly discuss possibile applications of the equation in modelling subdiffusion–reaction processes in biological systems.

REFERENCES

[1] Kosztołowicz T.: *Cattaneo–type subdiffusion–reaction equation*, arXiv:1306.3806, http://arxiv.org/abs/1306.3806 (18.06.2013), 1–10.