The modeling of anomalous transport in the diffusion-ballistic regime

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Abstract. The anomalous transport of a point-like particle within the disordered heterogeneous medium with accelerating traps was investigated using Monte Carlo simulation within the CTRW model. Outside the traps a particle moves according to the diffusion regime of motion. Inside the traps the ballistic regime takes place. Results of the Monte Carlo simulation shows that the final distribution of particle jumps belongs to the class of the stable distributions which corresponds to the anomalous diffusion regime. It is shown that the characteristic exponent of the stable distribution depends on the trap density and particle velocity inside the traps.

1. Introduction

In recent years the anomalous diffusion attracts the increasing interest in the research of diverse physical phenomena: delayed neutrons [1], cardiovascular systems [2], proteins transport in living cells [3] etc. In the first instance this interest is caused by the circumstance that structural features of the environment may be the reason of the anomalous transport [4]. Therefore a lot of works dedicated to the anomalous diffusion are focused on the diffusion in disordered media [5-10]. Such anomalous processes frequently appear within heterogeneous media because of the difference in velocity of particle motion in each phase. They are connected with acceleration (or deceleration) of a particle in media. For today a set of works are known in which the anomalous diffusion is studied in different heterogeneous systems: hindered transport of proteins in cell structures [3], cooling of silicon semiconductors, fast transport through CNT membranes [5] etc. Consequently the structural features of the medium and velocity of a particle inside the medium may determine the transport regime of particles.

Numerical simulations are frequently used for determination of the transport regime [6-10]. Various diffusion regimes (from sub-diffusion to ballistic) were obtained using numerical simulation for media with obstacles of different geometric shapes. Various objects, considered as obstacles and placed in a medium, were studied: spheres [6], rods, solid sphere and a permeable shell - a sphere of a larger radius (within so-called cherry-pit model [7]), a model of a porous medium formed with Voronoi tessellation [6, 8, 9], various lattice configurations with obstacles [10] etc. Lattice models are relatively simple to calculate and very well studied. Continuum models, on the contrary, are more complex in terms of modeling, however, they better describe real media - for example, polymers. Therefore, recently, continuous medium models are more often used. In these models transport processes can be described using the CTRW model [11]. CTRW makes it possible to describe jump
stochastic processes in terms of probability density functions (PDFs) of length of particle jumps and waiting time between them. A lot of processes with different probability density functions of times and jumps were considered and described within the CTRW model [12-18]. At the same time, these PDFs might not be always known initially. The question is how to describe the anomalous diffusion in systems where the PDF of jumps and/or times isn't known a-priori. The answer can be obtained from a numerical modelling.

In this work we present the results of modeling of the two dimensional heterogeneous medium with rectangle shaped traps with a solid core and a permeable shell (as a cherry-pit model). Outside the trap particle motion is the ordinary diffusion with jumps and jump times distributed by the Gauss and the Poisson PDFs, respectively. Particle motion inside a trap represents the ballistic regime -- after getting inside a trap a particle moves to the opposite side of the trap. Time of flight inside the trap was calculated from the fixed particle velocity inside the trap and the distance of flight. The results of modeling shows that the PDF of particle jumps in such heterogeneous medium corresponds to the stable distributions. A characteristic exponent of the stable PDF is determined by the density of traps and decreases characterized by the increase in trap density.

2. Numerical modeling
Calculations were performed on a square system with the linear dimension $L = 15$ within periodic boundary conditions. The system is randomly filled with rectangles. All rectangles have an impermeable solid core with dimensions $l = 1$, $d = 0.05$, and a permeable shell with dimensions $l = 1.05$, $d = 0.1$. The density of the rectangles is defined as $\eta = \frac{mN}{L^2}$, where $l, m$ is the length and the width of the rectangle, respectively, and $N$ is the number of rectangles. Density was varied in the range of $0 \leq \eta \leq 0.66$. For each density calculation was performed using the Monte Carlo method.

For each step of simulation there are two possible situations: the particle is located in the medium outside the trap or captured into the trap. Outside the trap particle motion is the ordinary diffusion and the space and the time steps are chosen from the Gaussian and the Poisson PDFs, respectively. When a particle attempts to jump into the area of impermeable rectangles, it is reflected from a solid core into the region of a permeable shell. If a particle belongs to one of the permeable rectangles (a particle is trapped), it moves to the opposite side of the rectangle. The flight time is calculated from the specified dimensionless velocity $V$ ($V = 100, V = 0.1$ and instantaneous displacements are investigated) and the distance corresponding to the flight length. For each simulation we calculated the final position of the particle at time $t = 10000$. Totally we performed $10^6$ simulations for each value of the trap density.

3. Analysis and results
We used the following parametrization of the stable distribution [19]:

$$\varphi(t, \alpha, \beta, c, \mu) = \exp \left[ i t \mu - |ct|^\alpha \cdot (1 - i \beta \cdot \text{sgn}(t) \cdot \tan \left( \frac{\pi \alpha}{2} \right) \right], \alpha \neq 1$$

Where $-\infty < \mu < \infty$, $c \geq 0$, $0 < \alpha \leq 2$, $-1 \leq \beta \leq 1$ are the distribution parameters.

The characteristic exponent $\alpha$ determines the form of the distribution function, location parameter $\mu$ - position of the maximum of the distribution, scale parameter $c$ - width of the distribution, and skewness parameter $\beta$ determines distribution asymmetry.

For $\alpha = 2$ the stable distribution changes into the Gaussian distribution. Since the main difference between the Gaussian and stable distributions corresponds to the characteristic exponent $\alpha$, we focused on its calculation. $\alpha$ was calculated using the maximum likelihood method. In our case, $1 < \alpha < 2$. 


Figure 1 shows the dependence of the characteristic exponent $\alpha$ on the trap density $\eta$ for the case of finite velocity and for instantaneous particle displacements in traps. In the absence of the traps ($\eta = 0$) characteristic exponent $\alpha = 2$ corresponds to the Gauss distribution, whereas for every $\eta > 0$ we obtain stable distribution with $\alpha < 2$. This result corresponds to the effective acceleration of the particle caused by traps and transition from the diffusion to the superdiffusion regime. Effect of the finite particle velocity in the traps slightly slows down the acceleration process in comparison with the case of instantaneous displacements, as shown in [20]. This slowdown is illustrated in Figure 1. It is seen that decreasing of the velocity corresponds to increasing of the characteristic exponent $\alpha(\eta)$.

This increasing corresponds to the decreasing of the mean square displacement of the particle during the walk in the heterogeneous medium. However, in spite of the fact that the finite velocity of motion slows down the particle in comparison with the case of instantaneous displacements, the form of the distribution of jumps in traps remains stable [20].

From Figure 1 it can be seen that the velocity impacts weakly on the parameter $\alpha$ for $\eta < 0.3$. However, when $\eta > 0.3$, change of speed has a significant impact on the shape of stable distribution showed on Figure 2. This effect may be associated with formation of the clusters of connected traps with increasing traps density: clusters create a path along which the particle will fly through the cluster and that increase the effective speed of movement. The formation of the connected traps through which ballistic transport takes place allows the particle to fly away on long distances, unlike the case of unconnected traps. Thus, two factors apparently influence on the mean square displacement of a particle: the formation of clusters of connected traps and the ballistic regime of motion. However, stable distributions are caused by the ballistic regime of motion inside the traps.
Figure 2. The distribution function of the mean square displacement of a particle for the velocities

\( V=0.1, \ V=10 \) for a fixed density \( \eta = 0.578 \).

4. Conclusions

In this paper the diffusion of a particle inside the heterogeneous media with accelerating traps has been investigated using the Monte Carlo method. A particle inside accelerating traps moves in the ballistic regime. The results of simulation show that the distributions of particle jumps belong to the class of stable distributions. Therefore we present one of the possible mechanisms how stable distributions in the heterogeneous media are formed. Also, the influence of the main parameters – trap density and particle velocity in traps, on the form of obtained stable distribution has been investigated.

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