DIFFUSION IN MULTISTATE CONFIGURATIONS

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Abstract. We study the random walk of a particle in one and two-dimensional discrete systems, which are generated either with steady probability of lattice site choice type or with the conditional probability of the lattice site choice type. The main aim of this work is to determine the diffusion coefficient for some special cases.

Diffusion in disordered system attracts much attention due to its importance in physical and chemical processes. Two limited cases are frequently considered to analyse the nature of diffusion in systems with random properties: the so-called annealed and quenched disorder. From the microscopic point of view particles jump randomly between allowed sites with rates depending on the nature of the system. These transition rates may fluctuate in time independent of the position of the particle (annealed disorder) or they may be assigned randomly to the sites or bonds of the lattice independent of time (quenched disorder). Both cases has already been analysed and many important results were found [1-3]. The quenched disorder approach is more appropriate when some topological disorder is present in material or a random energy landscape generates quenched transition rates.

1. Diffusion in one-dimensional systems

Steady probability of the lattice site type. First we consider a random-walk model of a particle on a linear chain, where a jump length 1 or 2 is assigned randomly to each lattice site with constant probability p_1, $p_2 = 1 - p_1$, respectively. We will call a site i a 1 site if a jump length equals 1 and a 2 side otherwise. If the particle stays at 1 site it can jump to one of the two nearest-neighbour sites, while if stays at 2 site, it can jump to one of two 2-neighbour sites. The particle jumps with equal probability ½ to the left or to the right. In this model we obtain for the mean-field diffusion coefficient $D = \frac{1}{2}(4\text{-}3p_1)$, which yields 1.25 for $p_1 = p_2 = 0.5$. From numerical calculations we obtain the average diffusion coefficient $D_{average} =$ $= 1.09367$.

Conditional probability of the lattice site type. Consider the linear chain with the conditional probability of the occurrence the lattice site type 1 or 2. We assume, that p is the probability of the occurrence the lattice site of type 1 (2) in *i*- this part of chain on condition that the lattice site *i-1* was of type 1 (2), whereas q is the probability of the occurrence the lattice site of type 1 (2) in *i*- this part of chain on condition that the lattice site *i-1* was of type 2 (1). The particle can jump to one of the two nearest-neighbour sites, if it stays at 1 site or it can jump to one of two 2-neighbour sites, if stays at 2 site. The numerical calculations were performed for values p changing from 0.05 to 0.95 with step 0.05. On the basis of these calculations we obtain the average diffusion coefficients for individual cases. For example for $p = 0.05$, $q = 0.95$, $D_{average} = 1.98467$, for $p = 0.5$, $q = 0.5$, $D_{average} = 1.11164$ and for $p = 0.95$, $q = 0.05$, $D_{average} = 0.775593$.

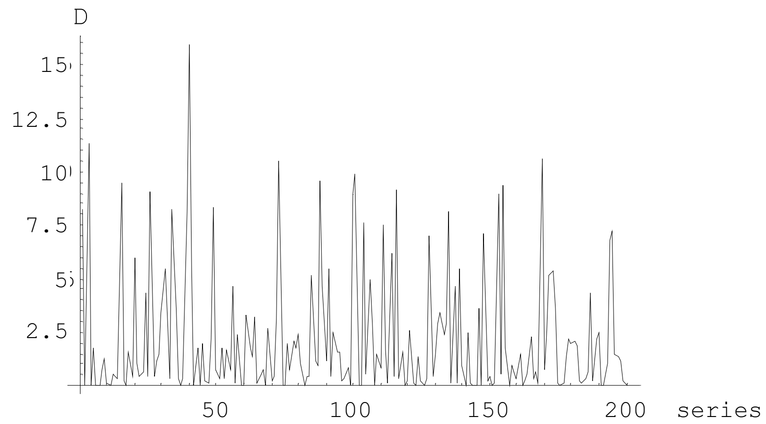

Fig.1. Diffusion of the particle after 1000000 jumps

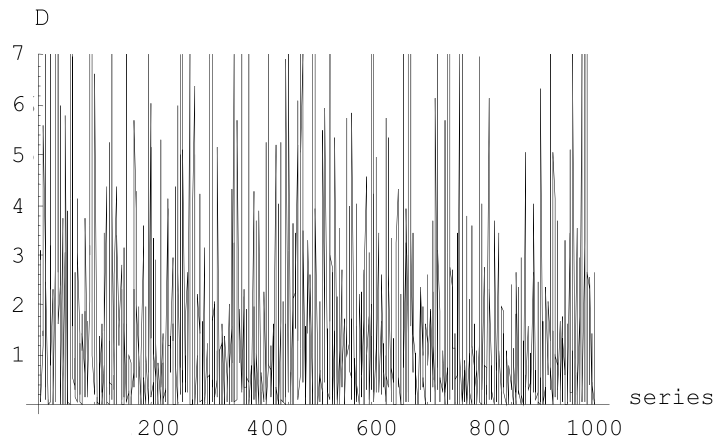

Fig. 2. Typical spectrum of the diffusion coefficient D for $p = 0.95$, $q = 0.05$

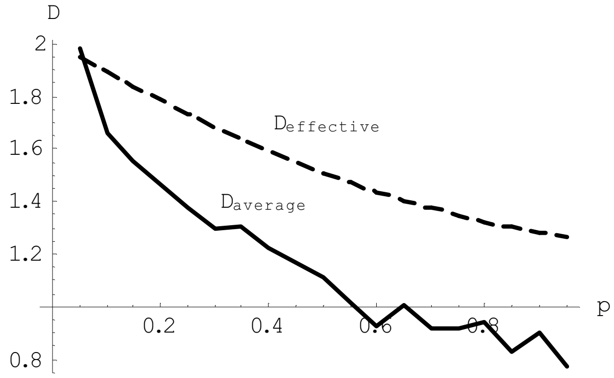

Fig. 3. Solid (dashed) line presents the changes of the average (effective, from analytical calculations) diffusion coefficient D as a function of the conditional probability value *p*

2. Diffusion in the two-dimension systems

Steady probability of the lattice site type. System contains two different types of the lattice site: type 1 with the probability p_1, type 2 with the probability $p_2 = 1 - p_1$. If moving particle stops in the lattice site 1, then in the next jump it can move to the one of the four neighbouring sites. In the case, when the particle finds itself in the lattice site type 2 moves about two knots. The movement of the particle is not directed. Numerical calculations gives the average diffusion coefficient $D_{average} = 0.3116$.

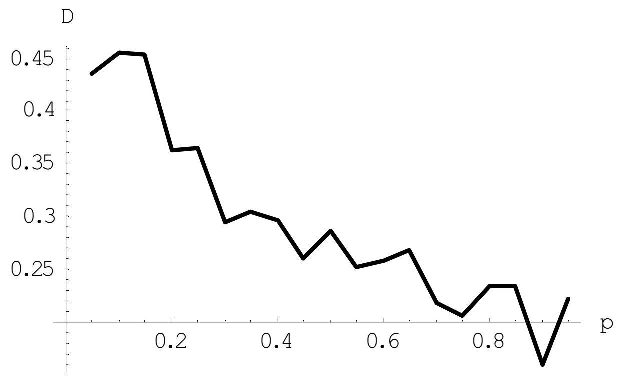

Fig. 4. Average diffusion coefficient depending on the conditional probability *p*

Conditional probability of the occurrence of the column of knots type 1 or 2. We assume, that *p* is the probability of the occurrence the column of knots of type 1 (2) in *i*- this column of system on condition that the column *i-1* was of type 1 (2), whereas *q* is the probability of the occurrence the column of knots of type 1 (2) in *i*- this column of system on condition that the column *i-1* was of type 2 (1).

The moving particle, like in previous case, if stops in the lattice site 1 then in the next jump it can move to the one of the four neighbouring sites. In the case, when the particle finds itself in the lattice site type 2 moves about two knots. The numerical calculations were performed for values p from 0.05 to 0.95 with step 0.05. On the basis of these calculations we obtained the average diffusion coefficients for these cases. For example for p = 0.05 and q = 0.95, $D_{average}$ = 1.98467.

In this paper we have analysed the influence of a quenched disorder given by a quenched jump length distribution on the diffusion properties of a particle inside of some special one and two dimensional systems. We have computed the values of the diffusion coefficient for some special cases of distribution of jump length.

References

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