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Anomalous diffusion in porous media

J. Prehl[1], K. H. Hoffmann[1], M. Hofmann[2], G. Rünger[2], S. Tarafdar[3]

[1] Department of Physics, Chemnitz University of Technology, Germany
[2] Department of Computer Science, Chemnitz University of Technology, Germany
[3] Condensed Matter Physics Research Centre, Jadapur University, India

Contact: {janett.prehl, hoffmann}@physik.tu-chemnitz.de

Abstract

We studied anomalous diffusion under the influence of an external force on finite regular Sierpinski carpets. In order to investigate the time development of the probability density $p(r,t)$ we utilize the master equation approach. Thus, we are able to determine important quantities depending on their space direction $e \in \{x, y\}$, like the mean drift velocities $\langle v_{\mathrm{dr}_e} \rangle$, the mean square displacements $\langle e^2 \rangle$ and the random walk dimensions d_{w_e}. Applying different force strengths in x-direction we find a maximum $\langle v_{\mathrm{dr}_x} \rangle$ for small to medium force strengths in x. According to $\langle x^2 \rangle \sim t^{\frac{2}{d_{\mathrm{w}_x}}}$, we determine that $d_{\mathrm{w}_x} < 2$ along the external force. So, diffusion seems to be superdiffusive, although diffusion is hindered by structure and delayed be waiting times. Finally, this seems to be the result of two competing effects. First, the particles get accelerated due to the external force. However, they get also trapped according to the complex structure which takes more time to escape caused by the external force. Thus, the distribution spreads faster with than without an external force and $d_{\mathrm{w}_x} < 2$.

1 Introduction

In technology and science we can observe many anomalous diffusion processes influenced by external forces. Examples are the impedance spectroscopy measurements as for polymer electrolytes [1], hopping electron conduction in doped semiconductors in strong electric fields [2], or diffusion of particles in gels under high gravity or centrifugal force as in chromatographic columns [3].
The external force causes diffusing particles to move preferred in direction of the external force direction. Besides, also the complex structure of real materials [4], like self-similarities of certain length scales, play an important role. We apply regular Sierpinski carpets (SC), a special kind of fractals, to model these complicate structures. SCs are defined by a generator, which is a square divided in $n \times n$ subsquares (see Fig. 1). There are m subsquares labeled black and the rest are white that means they are removed. In order to construct a SC we start with a generator and in each iteration step we replace every black subsquare by a scaled down version of the generator. If this is repeated ad infinitum, the limit object is a SC, where we define its fractal dimension d_{f} as $d_{\mathrm{f}} = \frac{\log m}{\log n}$. As real materials have a smallest length scale of self-similarity, we stop the iteration process after l times and we obtain an iterator of depth l. Furthermore, we combine copies of the iterator to one carpet. Thus, we model the effect that disordered media are rather homogeneous at large length scales [5].
It is known that such complex structures lead to anomalous subdiffusion [6]. So the mean square displacement $\langle r^2(t) \rangle$ of diffusing particles increases not linear in time t, as for normal diffusion, but

$$\langle r^2(t) \rangle \sim t^{\frac{2}{d_{\mathrm{w}}}}, \tag{1}$$

where $d_{\mathrm{w}} > 2$ is the random walk dimension [7].
In the next section we will introduce our simulation model and the chosen parameters. Afterwards, we present our results and we will discuss them. Finally a short conclusion is given.

2 Diffusion model in disordered media

We model the diffusion on SCs with the master equation approach. With this approach we are able to calculate the time evolution of the probability density $p(r,t)$ of many particles or random walks on SCs. Analyzing the resulting $p(r,t)$ we can determine many important quantities depending on their space direction $e \in \{x, y\}$, as the mean drift velocities $\langle v_{\mathrm{dr}_e} \rangle$, the mean square displacements $\langle e^2 \rangle$ and thus, the random walk dimensions d_{w_e}, and many more.
The probability density $p(r_i, t)$ describes the probability p of a walker to be at time t at a certain position $r_i = (x, y)$. The new $p(r, t+1)$ can be calculated as

$$p(r_i, t+1) = \Gamma_{ii} p(r_i, t) + \sum_{j \in \langle i \rangle} \Gamma_{ij} p(r_j, t), \tag{2}$$

where $j \in \langle i \rangle$ represents all neighboring black squares r_j of r_i, Γ_{ij} is the transition probability for a walker to move from square r_j to r_i and Γ_{ii} is the probability to stay. We choose our transition probabilities according to the blind ant model [8]. That means every

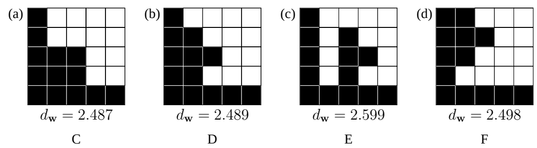

Fig. 1: *Four different generator patterns with same* $d_f = 1.59$

neighboring square is chosen with a probability of $1/4$. If there is a neighboring black square, Γ_{ji} is set to $\Gamma_{ji} = 1/4$. The walker stays on its current position with a probability $\Gamma_{ii} = 1 - \sum_{j \in \langle i \rangle} \Gamma_{ji}$, if there is white square.
We modified the transition probabilities according to the external force, we want to apply [9]. Thus, we defined a vector $\underline{b} = (b_x, b_y)$ with $b_x, b_y \in [0 : 1]$ for the external force strength. So our new transition probabilities to neighboring black squares are

$$\Gamma_{ij} = \frac{1}{2d} \left(1 + \underline{e}_{ji} \underline{b}\right), \tag{3}$$

with d as space dimension and $\underline{e}_{ji}$ as unit vector pointing to the four neighboring squares r_j.
Implementing the master equation approach requires an efficient processing of large data sets. In every time step we need to calculate the probabilities $p(r_i, t+1)$ for all squares r_i using the probabilities of the previous time step and the neighboring information of the SCs. The irregular carpet structure requires appropriate data structures and efficient algorithms for querying, calculating and storing all necessary data. Because of the high computational workload and the memory requirements, a parallel implementation based on the Task Pool Teams concept [10] was used to solve the master equation on regular and randomized SCs .

3 Results and discussion

We applied four different generator patterns, shown in Fig. 1, with same fractal dimension d_f but different random walk dimension d_w, in order to analyze effects of structures like dead ends to the diffusion influenced by an external force, like temperature difference, magnetic or electric fields. The external force is chosen to be along the positive x-axis. We investigated two important quantities for different iteration depths $l = 1, 2, 4$. But, we will present all results for $l = 2$, and in first order for generator E, as time scales and structure elements are appropriate to show and to discuss all necessary phenomena, however they appear in all iteration depths. We calculated the drift velocities $\langle v_{\mathrm{dr}_e} \rangle$ and the second central mean square displacements $\langle D^2(X_e) \rangle = \langle e \rangle^2 - \langle e^2 \rangle$, both in x- and y-direction, and depending on the external force.
First, we present our results of the drift velocity $\langle v_{\mathrm{dr}_e} \rangle$ over the external force strength b_x for the generators C, D, E, and F (see Fig. 2). We know that for homogeneous media we find a monotonic increasing $\langle v_{\mathrm{dr}_x} \rangle$ for increasing b_x. However, in Fig. 2(a), we see a non-monotonic response of $\langle v_{\mathrm{dr}_x} \rangle$ for increasing b_x [9, 11]. We observe a maximum $\langle v_{\mathrm{dr}_x} \rangle$ for small to medium amplitudes. Perpendicular to the force, in y-direction (Fig. 2(b)), we

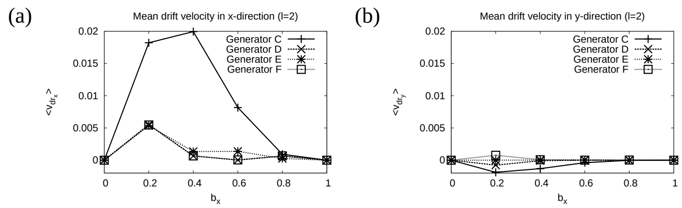

Fig. 2: *Here the mean drift velocities $\langle v_{\mathrm{dr}_e} \rangle$ in x- and y-direction for different force strengths b_x are shown for all generators (see Fig. 1).*

find such a non-monotonic behavior for $\langle v_{\mathrm{dr}_y} \rangle$ at smaller order of magnitudes. But, this small drift is caused by the fractal structure of the medium, where diffusion takes place.
Then we analyze the time development of the mean square displacement $\langle D^2(X_e) \rangle$, which can be seen in Fig. 3 for generator E. The vertical lines in the graph represent the average number of time steps $t_1 = 4298$ and $t_2 = 281753$ to cross the linear size of an iterator of depth $l = 1$ and 2. Furthermore, we also introduce a reference graph for normal diffusion ($d_\mathrm{w} = 2$).
In Fig. 3(a), we observed that along the external force and within the fractals regime ($t < t_2$) the slopes of $\langle D^2(X_x) \rangle$ are steeper than normal diffusion, thus $d_{\mathrm{w}_x} < 2$. This corresponds to superdiffusion. On the other hand, we find that without an external force ($b_x = 0$) and perpendicular to the force (see Fig. 3(b)) the slopes are flatter than normal diffusion, so $d_{\mathrm{w}_y} > 2$ and subdiffusive behavior can be seen. In all cases we recognize that diffusion crosses over to normal diffusion for long time scales ($t > t_2$).
Although diffusion is hindered by structure and particles get trapped in dead ends we observe a superdiffusive behavior along the external force. In order to analyze that phenomena we determine the marginal distribution $\tilde{p}(x,t) = \sum_y p((x,y),t)$ of $p(r,t)$. We plotted $\tilde{p}(x,t)$ over x (Fig. 4) for generator E at time $t = 489$ for $b_x = 0$ and $b_x = 0.4$. The vertical line represents the mean value $\langle x \rangle$ of $p(r,t)$.
For $b_x = 0$, we see that $\langle x \rangle$ is close to the maximum peak of $\tilde{p}(x,t)$ at the position $x = 0.79$. Moreover, the distribution is fast decaying to both sides similarly. However, applying an external force $\langle x \rangle$ and the main peak of $\tilde{p}(x,t)$ are not at the same position. Furthermore, we do not observe only one major peak, but three and the whole distribution

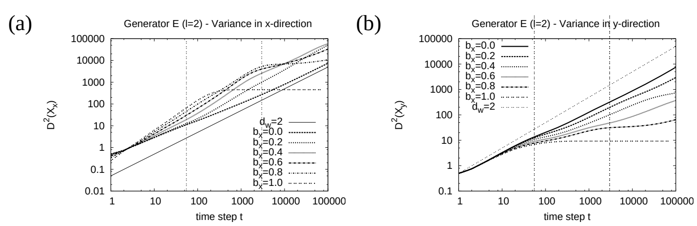

Fig. 3: *It is presented the central mean square displacement $D^2(X_e)$ in x- and y-direction over time t for an iterator of depth $l = 2$ of generator E (see Fig. 1(c)).*

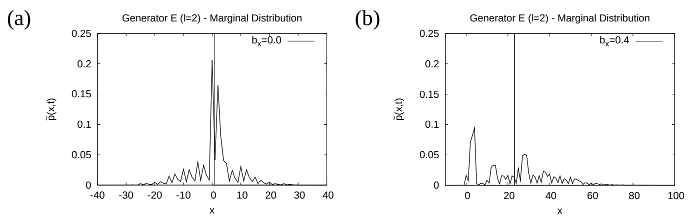

Fig. 4: *The marginal distribution $\tilde{p}(x,t)$ over x is shown for generator E ($l = 2$) (see Fig. 1(c)) for $b_x = 0.0$ and $b_x = 0.4$.*

is flatter for $b_x = 0.4$ than for $b_x = 0$.
That means, particles follow two competing effects. First they move preferred and thus faster along the external force. But they still get trapped according to the structure. If the traps lay along the force direction, it takes more time to escape. The distribution flattens down much faster and $d_{\mathrm{w}_x} < 2$. So, we see an overlapping of subdiffusion, trapping and ballistic motion.

4 Conclusions

We studied anomalous diffusion on regular SC structures under the influence of an external force. Therefore, we investigated four different generator pattern with six different external force strengths applied at iteration depth $l = 2$.
We determined the probability distribution $p(r,t)$ and thus, the mean value $\langle x \rangle$, mean drift velocities $\langle v_{\mathrm{dr}_e} \rangle$ and central mean square displacements $\langle D^2(X_e) \rangle$ in x- and y-direction ($e \in \{x, y\}$). We found a non-linear response of $\langle v_{\mathrm{dr}_x} \rangle$ with increasing force strength in x-direction and we obtained maximum $\langle v_{\mathrm{dr}_x} \rangle$ for small and medium forces. Moreover, we observed $d_{\mathrm{w}_x} < 2$ along the external force. That implies a superdiffusive process, although diffusion is hindered by dead ends and waiting times.
An explanation gave us the analysis of the corresponding marginal distributions $\tilde{p}(x,t)$. We observed that particles undergo two competing effects, the acceleration due to the external force and a stopping and waiting corresponding to the trapping in dead ends along the external field. Thus, the distribution spreads and flattens much faster. So, d_{w_x} is larger than the 'normal' subdiffusional process on fractals and even larger than normal diffusion.

References

[1] M. Maitra, et al., Physica A, **346**, 199 (2004)

[2] H. Böttger, et al., Phil. Mag. B, **42**, 297 (1980)

[3] L. Fischer, *An introduction to gel chromatography* (North-Holland Publishing Company, Amsterdam, 1971)

[4] B. B. Mandelbrot, *The fractal Geometry of Nature* (W. H. Freeman and Company, New York, 1983)

[5] S. Tarafdar, et al., Physica A, **292**, 1 (2001)
[6] S. Havlin, et al., Adv. Phys., **36**, 695 (1987)
[7] A. Franz, et al., Fractals, **8**, 155 (2000)
[8] P. G. de Gennes, La Recherche, **7**, 919 (1976)
[9] J. Balg, *Diffusion on Fractals*, (http://archiv.tu-chemnitz.de/2007/0103/, Chemnitz, 2006)
[10] K. H. Hoffmann, et al., in W. E. Nagel, et al., eds., *Euro Par 2006, Parallel Processing* (Springer, Berlin, 2006)
[11] H. Böttger, et al., phys. stat. sol. (b), **113**, 9 (1982)