Random walks with feedback on fractal lattices

Beatrix M. Schulz* and Michael Schulz
Abteilung Theoretische Physik, Universität Ulm, D-89069 Ulm, Germany

Steffen Trimper†
Fachbereich Physik, Martin-Luther-Universität, D-06099 Halle, Germany
(Received 20 March 2002; published 27 September 2002)

We study numerically a random walk under the competitive processes of a self-organized feedback coupling, characterized by a strength λ and an underlying fractal lattice. Whereas a fractal structure favors a subdiffusive behavior, a dynamical feedback leads either to localization in case of an attractive feedback, $\lambda > 0$, or to superdiffusion for a repulsive memory strength $\lambda < 0$. Under the influence of both processes the dynamical exponent z is changed. For a Sierpinski gasket or a Sierpinski carpet with repulsive feedback coupling we get $2/z = 1.04$ or $2/z = 1.08$, respectively. When an attractive feedback is dominant, the system offers localization as in the case of a random walk in regular lattices. The numerical results are strongly supported by analytical studies based on scaling arguments.

DOI: 10.1103/PhysRevE.66.031106 PACS number(s): 05.40.−a, 05.45.Df, 61.43.Hv, 64.60.Ak

I. INTRODUCTION

Anomalous diffusion can be attributed to various reasons. From a more mathematical point of view, either anomalous diffusion is related to Lévy flights with a well defined power law distribution of waiting times and jump lengths or the diffusion is realized on a fractal lattice, for instance, on an infinite cluster close to the percolation threshold. Obviously, stochastic force fields are also able to generate anomalous diffusion below a critical dimension d_c [1,2]. Instead of a spatial varying random force term, a feedback coupling due to a memory of a random walker to its local environment at a previous time can be likewise the reason for anomalous diffusion. That case had been discussed by an analytical approach based on a renormalization group calculation [3]. The results could be confirmed by numerical simulations [4,5]. Furthermore, the numerical simulations are able to give more information than the one-loop renormalization group approach. In particular, one could find the crossover region from conventional diffusion to the memory dominated behavior. We get also a confirmation for the occurrence of localization, which has been argued within the renormalization group approach for by a runaway situation leading to a dynamical exponent $z \to \infty$, compare Eq. (1). Moreover, the simulation yields even a clear indication for logarithmic corrections expected at the critical dimension $d_c = 2$. The asymptotic behavior of the mean-square displacement is governed by a power law

$$\langle r^2(t) \rangle \sim t^{2/z}. \tag{1}$$

The mean-square displacement of the walker, averaged over many configurations and starting points, is mainly characterized by the exponent z. The exponent is changed due to the presence of the feedback coupling. If $1 < z < 2$ the transport is superdiffusive, meaning that the averaged square displacement grows faster than conventional diffusion. In the opposite case the process may be subdiffusive determined by an exponent $z > 2$, the random walk becomes slower. In according to the renormalization group results the numerical approach gave rise to a superdiffusive behavior with an exponent $z = 4/3$ in a one-dimensional space, $d = 1$. Based on a one-loop approximation within an $\epsilon = 2 - d$ expansion, it gives [3]

$$\frac{2}{z} = 1 + \frac{2-d}{2}. \tag{2}$$

Such a behavior is observed in case of a negative feedback-coupling strength $\lambda < 0$, see Eq. (4) below. Such a repulsive memory means that the walker tends to prevent previously visisted regions. If the feedback is attractive, $\lambda > 0$, both the numerics [4,5] as well as the renormalization group method [3] offer localization, i.e., after a certain initial time the mean-square displacement remains constant or with other words the dynamical exponent (1) is $z \to \infty$. Let us stress that our approach with a feedback coupling bears resemblance to the true self-avoiding walk considered successful in the 1980s by several authors [6,7]. In the model a traveler had been studied who steps randomly, however, avoiding sites visited already. Different from that approach we have enclosed an additional feedback in or approach to mimick the memory effects. The feedback is nonlocal in times and, furthermore, determined in a self-organized manner by the probability to find a traveler at a certain spatial point at a certain time. Therefore it seems to be worth considering a combination between feedback coupling and fractality of the underlying spatial structure. The random walk on fractals is widely discussed in a diverse variety of physical situations ranging from growth phenomena in both regular and disordered systems, to heterogeneous catalysis and other chemical reactions and to applications in biology and medicine. The literature is quite extensive and includes several books [8–11]. Due to the presence of large holes, bottlenecks, and

*Electronic address: beatrix.schulz@physik.uni-ulm.de
†Electronic address: trimper@physik.uni-halle.de

dangling ends in the fractals, the motion of a random walker is slowed down on all length scales [8]. Instead of Eq. (1) the mean-square displacement is described by a new exponent d_w, the walker exponent, defined by

$$\langle r^2(t)\rangle \sim t^{2/d_w}. \tag{3}$$

The fractal dimension of the random walk d_w is always greater than 2 indicating subdiffusive behavior. Whereas in a recent study [12] the authors have discussed self-avoiding walks on Sierpinski lattices in two and three dimensions, we present simulations on those fractal structures under the inclusion of feedback effects which lead in the special case of a repulsive feedback to the so-called true self-avoiding walk [6,7]. In doing so we are faced with a competition between the tendency to slow down the motion due to the fractality and to an acceleration due to a repulsive memory. For that reason we extend our previous simulations [4,5] by considering the random walk on a fractal lattice. In case of an attractive feedback both effects, the hopping process on a fractal as well as the feedback, tend to cause a slowdown of the motion. Therefore, one should expect more pronounced localization effects. In the opposite case of a repulsive feedback strength, leading to a superdiffusive behavior on a regular lattice, the dynamical exponent z for the diffusion on a fractal lattice is determined by two conflicting processes, an acceleration originated by the memory and a slowdown due to the underlying fractal structure. Therefore, it is our aim to measure the exponent z to decide which effect is the dominant one. Physically, this phenomena can be expected in case of the cation diffusion in glasses that offer a strong memory [13]. Accordingly, diffusion in glasses is discussed as an intrachannel hopping on fractal-like networks. Furthermore, such a behavior can be observed likewise in porous media [14].

The aim of the present paper is to verify the competition between anomalous diffusion effects caused by several phenomena, namely, subdiffusion induced by fractal spatial structures and either superdiffusion or even localization, originated by the above mentioned memory effects. The reason to focus the study on deterministic fractals is twofold. On one hand such fractals allow to minimize the finite size effects within the numerical approach, and on the other hand the results can be directly compared with those obtained for the self-avoiding walks on the Sierpinski lattices [12].

II. ANALYTICAL APPROACH

An analytical approach for a random walk under the influence of feedback effects based on a generalized Fokker-Planck equation, recently proposed by [3]. The nonlinear equation with memory effects, known as the Nakajima-Zwanzig equation [15], can be derived by applying a suitable projection operator on the total probability distribution in the phase space [16]. Introducing $P(\mathbf{r},t)$ as the probability density to find a particle at time t in an interval around the spatial point $\mathbf{r}$ the evolution equation for the single-particle distribution reads

$$\partial_t P(\mathbf{r},t) = D\nabla^2 P(\mathbf{r},t) - \lambda \int_0^t P^2(\mathbf{r}-\mathbf{r}',t-t')\partial_{t'} \times P(\mathbf{r}',t')d^d r' dt'. \tag{4}$$

In deriving the form of the memory term we are following a line given first in [17]. Generally, the memory term in the Nakajima-Zwanzig equation can be written as $\int K(\mathbf{r}-\mathbf{r}',t-t')\partial_{t'}P(\mathbf{r}',t')d^d r' dt'$. To proceed we have adopted arguments of the mode-coupling approach by which progress had been achieved in explaining various phenomena in the vicinity the glass transition of supercooled liquids [18,19]. As the main assumption we suppose that the memory is self-organized by all the other particles of the system which behave in the same manner as the one under consideration. Therefore, the relevant time and spatial scales of the memory should be essentially determined by the probability density $P(\mathbf{r},t)$ itself. Expanding the memory kernel with respect to P, the most relevant term is given by $K(P) \simeq P^2$ according to the mode-coupling theory [17–20]. Higher order terms can also occur but they are irrelevant in the renormalization group approach [3]. Due to the feedback coupling, manifested by the memory term in Eq. (4) the motion of a single particle is influenced apparently. The probability to find a certain particle at the point $\mathbf{r}$ at time t is also determined by the probability to observe the particle in the surroundings prior to the actual observation at t. The influence of the feedback term can be estimated. If the particle offers the tendency to leave the spatial point $\mathbf{r}'$ at time t', i.e. $\partial_{t'}P(\mathbf{r}',t')<0$, then an attractive memory coupling strength $(\lambda>0)$ enhances the probability at $P(\mathbf{r},t)$. A positive memory strength favors the return of the particle to a certain point during a sufficiently long time interval. In the opposite case, a negative memory $(\lambda<0)$ should prevent strongly the return to a site initially occupied. As discussed above, the basis mechanism is similar to true self-avoiding walk [6,7]. However in our approach the memory kernel is defined via the quantity $P(\mathbf{r},t)$ itself and, moreover, the behavior of the system is discussed depending on the sign of the feedback term. It results in either superdiffusion for a repulsive feedback term or alternatively subdiffusion or localization in case of an attractive memory. Such a behavior had been observed in more detail by applying a dynamical renormalization group approach [3]. As the result the authors found a superdiffusive behavior in case of a repulsive memory strength, $\lambda<0$, where the dynamical exponent is given by Eq. (2). For an attractive memory, $\lambda>0$, the renormalization group approach suggested localization characterized by $z\to\infty$. As already stressed before, simulations on a regular lattice have supported the analytical results [4,5]. Now, we extend the analysis by including fractal lattices. Because an analytical approach is not available up to now we have made numerical simulations. Before we present the results, let us estimate the influence of the fractality of the lattice. To that aim we have to discuss a relation between the walker exponent d_w, see Eq. (3) and the exponent z in Eq. (1), which is determined by the spatial dimension, compare Eq. (2). On a fractal lattice it should be a reasonable approximation to replace the dimension d in Eq. (2) by the fractal dimension d_f. Transport on a fractal lattice can be interpreted as transport with an effective waiting time, i.e., the time scale has to be rescaled to eliminate such waiting time effects. Introducing a new time scale according to

$$T = t^{2/d_w}, \tag{5}$$

we get

$$\langle r^2 \rangle \sim t^{2/d_w} \sim T. \tag{6}$$

The assumption that on the new time scale the mean-square displacement is similar to that of a random walk on a regular lattice leads to $\langle r^2 \rangle \sim T$. Considering the dynamical exponent under the inclusion of a memory as $z = z_m$, given by Eq. (2), the memory effect can be described by a further scaling law by which the mean-square displacement will be related to the new time scale: $\langle r^2 \rangle \sim T^{2/z_m}$. Combining Eqs. (2), (5), and (6) we find $\langle r^2 \rangle \sim t^{2/z}$ with

$$z = \frac{d_w}{1 + \frac{2 - d_f}{2}}. \tag{7}$$

As explained above we have replaced the dimension d by the corresponding fractal dimension d_f. Based on the last relation we can estimate the expected values of z for different fractal lattices. For instance, a Sierpinski gasket is characterized by $d_f = \ln 3/\ln 2$. The walker dimension is $d_w = \ln 5/\ln 2$. From here we conclude a dynamical exponent $z = 1.9221$ or

$$\frac{2}{z} = 1.0405. \tag{8}$$

The same estimation for a Sierpinski carpet, sometimes denoted as Menger sponge when embedded in a $d=3$ matrix, with the fractal dimension $d_f = \ln 8/\ln 3$ and $d_w = \ln(28/3)/\ln 3$ leads to $z = 1.9296$ or

$$\frac{2}{z} = 1.0365. \tag{9}$$

In the following section we will test the conjecture of Eq. (7) using numerical simulations.

III. NUMERICAL APPROACH

In this paper we focus our attention on the diffusion on deterministic fractals. Especially, we use the Sierpinski gasket and the Sierpinski carpet for our simulation to minimize finite size effects. In principle, the numerics can be extended to more refined structures as random fractals or treelike ones. However, the main goal of the paper is to study the competition between the subdiffusive behavior originated by the fractality and the superdiffusive effects due to the feedback mechanism. Here, we adopt the method recently applied for simulations on regular lattices [4,5] to fractals. The motion of the tracer particle is defined by a series of discrete jumps in discrete time intervals. The feedback coupling is introduced by marking each visited lattice bond by a certain number that accumulates all previous visits of that bond. The number, called the local visiting number, is used as a measure for the probability of a renewed visit of the same lattice bond. Whereas in case of a positive feedback coupling (attraction) the probability becomes higher with increasing number of visits, it decreases if the memory strength is negative or repulsive. Using the elementary time step $\delta\tau$, the discrete time scale is given by $t = n\,\delta\tau$ ($n = 0,1,2,\ldots$). The diffusion is now defined by randomly chosen jumps between neighbored fractal lattice sites after each discrete time step. To include the memory effects, let us define local visiting numbers b_{ij} characterizing the bonds between the neighbored lattice sites i and j. The transition rates from i to j and from j to i, respectively, for a particle are given by

$$t_{ij} = \frac{b_{ij}}{\sum_{k(i)} b_{ik}} \qquad \text{and} \qquad t_{ji} = \frac{b_{ji}}{\sum_{k(j)} b_{jk}}, \tag{10}$$

where $k(j)$ means summation over all nearest neighbors k of the lattice site i. Thus, $\Sigma_{k(i)} t_{ik} = 1$, i.e., the total probability for a jump of a particle is always 1. The initial values of the b_{ij} are given by $b_{ij} = 1$ for all neighbored fractal lattice sites. If the visiting numbers remain unchanged, one obtains a simple fractal random walk. To obtain a memory effect, we introduce a self-induced change of the visiting numbers, which causes the feedback of the particle on the environment. That means, the quantity b_{ij} now becomes time dependent. After each time step we redefine the local visiting number using the rules

$$b_{ij}(t + \delta\tau) \neq b_{ij}(t)$$

if the actual jump crosses the bond between i and j,

$$b_{ij}(t + \delta\tau) = b_{ij}(t) \quad \text{if the actual jump crosses another bond.} \tag{11}$$

The first rule must be specified: a positive memory is defined by a change $b_{ij}(t+\delta\tau) > b_{ij}(t)$, a negative memory requires $b_{ij}(t+\delta\tau) < b_{ij}(t)$. These time dependent visiting numbers break the local symmetry of the transition rates, i.e., the rates for jumps from a given point to neighbored sites may be differ after sufficiently long time. Clearly, a multiple crossing of a bond leads to an accumulation effect which increases (or decreases) the local visiting numbers remarkably, also if $|b_{ij}(t+\delta\tau) - b_{ij}(t)| \ll b_{ij}(t)$. It can be expected that this accumulation supports the generation of a (self-induced) localization (in the case of a positive memory) or a superdiffusion (negative memory). This memory effect superposes the anomalous diffusion due to the fractal structure of the underlying lattice. The final character of the diffusion in the case of a fractal subdiffusion and superdiffusional memory effects is determined by their strengths.

IV. RESULTS

A. Superdiffusion

We use the following quantitative rule: each crossing of a bond (ij) by the particle changes the corresponding visiting

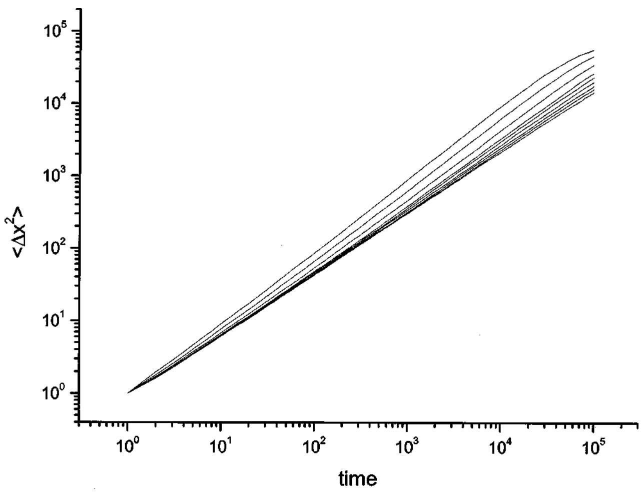

FIG. 1. Averaged mean-square displacement for a repulsive memory with strength $\varepsilon=0.0001,0.007,0.02,0.04,0.07,0.1,0.2,0.4,0.7$ (bottom up) on a Sierpinski gasket with $d_f=\ln 3/\ln 2$ and $2/z=1.04$. The deviations at the long time limit are caused by finite size effects.

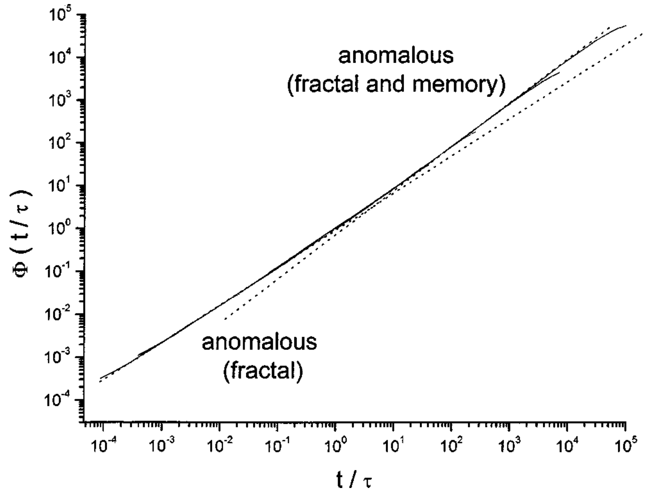

FIG. 3. Master curve of the mean-square displacements depicted in Fig. 1 with negative feedback. The collapse of all curves indicates strongly a universal behavior.

number via $b_{ij}\to b_{ij}(1-\varepsilon)$, with the feedback parameter $0<\varepsilon<1$. Here, the quantity ε is a measure for the memory strength. Such a relation generates a negative memory $\lambda(\varepsilon)$. The control parameter ε determines the coupling between particle and environment ($\varepsilon=0$ corresponds to pure fractal diffusion). We expect that each $\varepsilon\neq 0$ leads always to a superdiffusive contribution to the anomalous fractal diffusion behavior. Thus, the numerical simulations were realized for various values of the quantity ε. In Fig. 1 we have depicted the mean-square displacement for a Sierpinski gasket with the fractal dimension $d_f=\ln 3/\ln 2$ and the walker dimension $d_w=\ln 5/\ln 2$. The same quantity is presented in Fig. 2 for a Sierpinski carpet with $d_f=\ln 8/\ln 3$ and $d_w=\ln(28/3)/\ln 3$. The determination of the time dependent mean-square displacement shows the original fractal diffusion for a short time interval and small values of the feedback parameter ε. After a well defined crossover time $\tau_{\mathrm{c,sup}}(\varepsilon)$ the superdiffusive regime is achieved with the universal exponent $2/z=1.04\pm 0.02$ for a Sierpinski gasket and $2/z=1.08\pm 0.02$ for the Sierpinski carpet, respectively. The dynamical exponents are in reasonable agreement with the estimations given by Eqs. (8) and (9) obtained by simple scaling arguments based on Eq. (7). Furthermore, a rescaling of time and coordinates leads to a collapse of all curves presented in Fig. 3 onto a scaling function Φ^-, i.e., we obtain the general representation

$$\langle \mathbf{r}^2\rangle=\rho^2(\varepsilon)\mathbf{\Phi}^-\left(\frac{t}{\tau_{\mathrm{c,sup}}(\varepsilon)}\right), \tag{12}$$

with $\Phi^-\simeq s^{2/d_w}$ for $s\to 0$ and $\Phi^-(s)\simeq s^{2/z}$ for $s\to\infty$. Such a

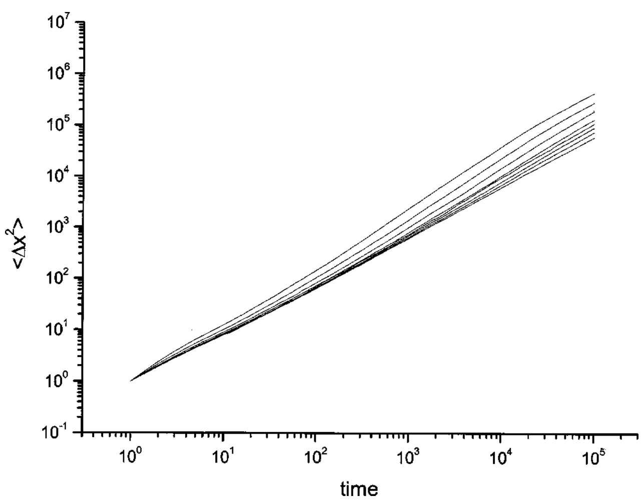

FIG. 2. Averaged mean-square displacement for a negative feedback strength $\varepsilon=0.0001,0.02,0.04,0.07,0.1,0.2,0.4,0.7$ (from the bottom up) on a Sierpinski carpet with $d_f=\ln 8/\ln 3$ and $2/z=1.08$.

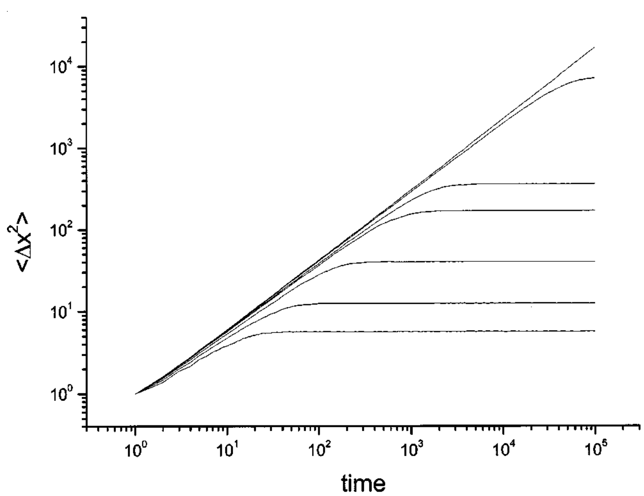

FIG. 4. Mean-square displacement for an attractive feedback on a Sierpinski gasket with $\varepsilon=0.0001,0.02,0.04,0.1,0.2,0.4,0.7$ (top down). It results in localization for a sufficiently long time interval.

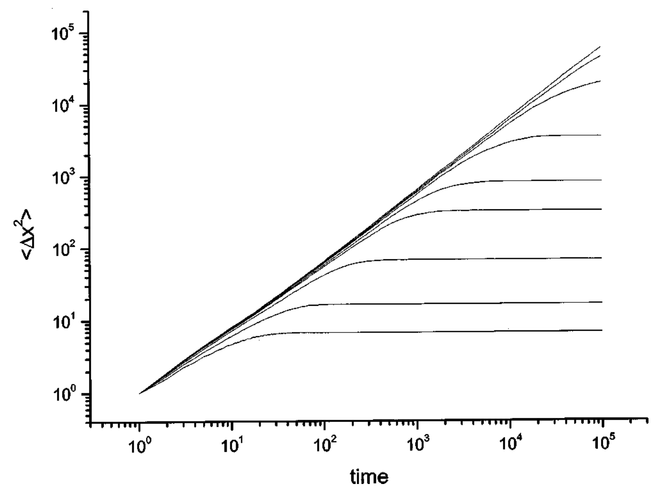

FIG. 5. Mean-square displacement for a positive feedback on a Sierpinski carpet with $\varepsilon=0.0001,0.01,0.02,0.04,0.07,0.1,0.2,0.4,0.7$ (top down), which always shows localization.

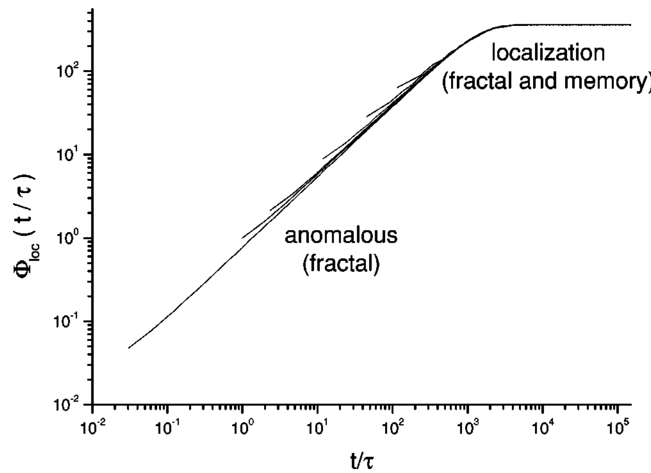

FIG. 6. Master curve of the mean-square displacements drawn in Fig. 4 with positive feedback strength.

behavior is observed in Fig. 3 for a Sierpinski gasket. A similar behavior can be obtained for the Sierpinski carpet.

B. Localization

In case of an attractive memory $\lambda(\varepsilon)$ the feedback is simulated by the rule $b_{ij}\rightarrow b_{ij}(1+\varepsilon)$ with $\varepsilon>0$. Both, the renormalization group approach [3] as well as the numerical analysis [4,5] gave evidence for a localization of the particle in a region around the initial position in case of using a regular lattice. In the present case the mean-square displacement offers likewise a fractal diffusive behavior in the short time regime. However after a crossover time $\overline{\tau}_{\mathrm{c,loc}}(\varepsilon)$ the curve approaches a constant value which indicates localization, see Fig. 4 for the Sierpinski gasket and Fig. 5 for the Sierpinski carpet, respectively. Both figures suggest a localization radius $\tilde{r}$ defined by $\lim_{t\rightarrow\infty}\sqrt{\langle\mathbf{r}^2\rangle}\sim\tilde{r}(\varepsilon)$. A rescaling of time and coordinates leads again to a collapse of all curves onto the scaling function Φ^{+}, i.e., we obtain the general representation

$$\langle\mathbf{r}^2\rangle=\tilde{r}^2(\varepsilon)\Phi^{+}\left(\frac{t}{\tau_{\mathrm{c,loc}}(\varepsilon)}\right), \tag{13}$$

with $\Phi^{+}(s)\simeq s^{2/d_w}$ for $s\rightarrow 0$ and $\Phi^{+}(s)=1$ for $s\rightarrow\infty$. This behavior is represented in Fig. 6 for the Sierpinski gasket. In our model we find $\tilde{r}(\varepsilon)=\tau_{\mathrm{c,loc}}^{d_w}(\varepsilon)$, where d_w is the walker dimension in case of pure fractal diffusion.

V. CONCLUSION

In the present paper we have extended previous studies on random walks in regular lattices under the influence of a self-organized feedback to random walks in fractal structures. In particular, the goal of our analysis had been to test the conjecture that the character of the feedback leads to a significant modification of the mean-square displacement in the asymptotic limit. We have demonstrated, using a numerical approach, that the diffusive behavior is changed drastically due to the underlying fractal lattice and the memory. The reason for that variation is a competition between time delay effects and the fractality. As far as the fractal dimension of the lattice d_f is smaller than a critical dimension d_c, the motion of a walker is strongly influenced by the memory as well as by the fractal properties. In case of a negative memory strength, which can be considered as a kind of repulsion for a walker, the combination of both memory effects and the fractal lattice lead to a superdiffusive behavior. Thus the feedback dominates the behavior of the system. When a particle, moving through a fractal lattice, is subjected to an attractive memory strength, it tends to come back to a lattice site visited already before. In this case that feedback coupling gives rise to localization characterized by a constant mean-square displacement in the time asymptotic limit. Whereas the walker offers diffusive behavior in the initial time interval there is a crossover to a feedback dominated regime, which indicates localization. In that case the feedback effects are so strong that the diffusion will be stopped and the particle becomes fixed on average within a finite spatial interval. Such a behavior should be of interest also in large percolation clusters in the vicinity of the percolation threshold or in growth processes in biological systems. A further extension of our approach should be the inclusion of disorder effects originated by external force fields or pinning effects within the lattice. Analytically, Eq. (4) could be generalized by including the fractional derivative operator as it had been discussed in recent papers, see, for instance, Ref. [21], where the evolution of the probability density is discussed using the fractional Fokker-Planck equation.

ACKNOWLEDGMENTS

We thank A. Heide and C. Pientschke for a fruitful collaboration concerning the numerical problems described here. We are very grateful to the Deutsche Forschungsgemeinschaft (Grant No. DFG-SFB 418) for financial support.

[1] D.S. Fisher, D. Friedan, Z. Qiu, S.J. Shenker, and S.H. Shenker, Phys. Rev. A **31**, 3841 (1985).
[2] V.E. Kravtsov, I.V. Lerner, and V.I. Yudson, J. Phys. A **18**, L703 (1985).
[3] M. Schulz, S. Stepanow, Phys. Rev. B **59**, 13 528 (1999).
[4] B.M. Schulz, S. Trimper, Phys. Lett. A **256**, 266 (1999).
[5] B.M. Schulz, S. Trimper, and M. Schulz, Eur. Phys. J. B **15**, 499 (2000).
[6] D.J. Amit, G. Parisi, and L. Peliti, Phys. Rev. B **27**, 1635 (1983).
[7] S.P. Obuhkov, L. Peliti, J. Phys. A **16**, L147 (1983).
[8] *Fractals and Disordered Systems*, edited by A. Bunde and S. Havlin (Springer, Berlin, 1991).
[9] *Fractals in Science*, edited by A. Bunde and S. Havlin (Springer, Berlin, 1995).
[10] T. Vicsek, *Fractal Growth Phenomena* (World Scientific, Singapore, 1989).
[11] D. Ben-Avraham and S. Havlin, *Diffusion and Reactions in Fractals and Disordered Systems* (Cambridge University Press, Cambridge, 2000).
[12] A. Ordemann, M. Porto, and H.E. Roman, Phys. Rev. E **65**, 021107 (2002).
[13] G.N. Greaves and K.L. Ngai, Phys. Rev. B **52**, 6358 (1995).
[14] A. Klemm, R. Metzler, and R. Kimmich, Phys. Rev. E **65**, 021112 (2002).
[15] G. Fick, and E. Sauermann, *Quantenstatistik Dynamischer Prozesse* (Akademische Verlagsgesellschaft, Leipzig, 1983) Vol. 1.
[16] H. Mori, Prog. Theor. Phys. **34**, 399 (1965).
[17] E. Leutheusser, Phys. Rev. A **29**, 2765 (1984).
[18] W. Götze, in *Liquids, Freezing and the Glass Transition*, edited by Hansen *et al.* (North-Holland, Amsterdam, 1991).
[19] W. Götze, J. Phys.: Condens. Matter **11**, A1 (1999).
[20] J.P. Bouchaud, L. Cugliandolo, J. Kurchan, and M. Mezard, Physica A **226**, 243 (1996).
[21] I.M. Sokolov, Phys. Rev. E **63**, 056111 (2001).