Eur. Phys. J. B **15**, 499–505 (2000)

THE EUROPEAN PHYSICAL JOURNAL B

EDP Sciences

Random walks in one-dimensional environments with feedback-coupling

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Received 16 September 1999 and Received in final form 27 December 1999

Abstract. Random walks in one-dimensional environments with an additional dynamical feedback-coupling is analyzed numerically. The feedback introduced *via* a generalized master equation is controlled by a memory kernel of strength λ the explicit form of which is motivated by arguments used in mode-coupling theories. Introducing several realizations of the feedback mechanism within the simulations we obtain for a negative memory term, $\lambda < 0$, superdiffusion in the long time limit while a positive memory leads to localization of the particle. The numerical simulations are in agreement with recent predictions based on renormalization group techniques. A slight modification of the model including an exponentially decaying memory term and some possible applications for glasses and supercooled liquids are suggested. The relation to the true self-avoiding is discussed.

PACS. 05.40.-a Fluctuation phenomena, random processes, noise, and Brownian motion – 05.20.Dd Kinetic theory – 64.60.Ht Dynamic critical phenomena

1 Introduction

Anomalous diffusion can be attributed to various reasons. From a mathematical point of view, either anomalous diffusion is related to Levi-flights with a well-defined power law distribution of waiting times and jump lengths or the diffusion process is realized on a fractal space, *e.g.* on an infinite cluster at the percolation threshold. Obviously, stochastic force fields are also able to generate anomalous diffusion below a critical dimension [1,2]. Additional to the random walk in an environment in which there is a spatially random drift term $\mathbf{F}(\mathbf{r})$ a feedback-coupling of the random walker to its local environment at a former time can be also the reason for anomalous diffusion. This alternative way had been recently proposed by one of us (M.S.) [6] within an analytical model and by applying a renormalization-group approach. Here, we will demonstrate that the analytical results based on an one-loop expansion can be confirmed by numerical simulations. Moreover, the numerics yields additional information about the crossover to the memory dominated case and leads to systematic corrections which are not included in the analytical approach. Furthermore, we apply several methods that can systematically overcome possible non-stationarities in the data, especially in case of a memory coupling.

Our model with the feedback-coupling bears a close resemblance to the true self-avoiding walk considered in the eighties by several authors [3,4], for a renewed approach see [5]. Different to those models we have enclosed an explicit feedback-coupling term which is non-local in times. As demonstrated both by analytical studies [6] and by our present numerical approach the feedback-coupling leads as well as to a modified diffusive behavior (with similar exponents, see below) and additional also to localization of the particle.

Motivated is this kind of analysis by considering glasses and glass-like materials. In particular, our method seems to be relevant for the explanation of various phenomena in the vicinity of the glass transition of a supercooled liquid [7], for a recent review see [8], or for the mixed mobile ion effect [9,10], compare also [11]. Recently, it had been pointed out that anomalous diffusion should be observed in glasses below a characteristic time scale [12].

Our simulations are strongly supported by the mode-coupling theory [7,8,13,14] which had indeed achieved progress within an analytical approach of glass dynamics. However, the applicability of the mentioned theory is not restricted to glasses but it should be also relevant for other dynamical processes where a feedback-coupling plays an decisive role. Therefore, let us summarize for further convenience the general ideas behind the mode-coupling concept. It based on the following steps:

(i) Starting from the deterministic equation of motions all irrelevant observables will be eliminated applying a suitable projection operator formalism; as a consequence, the correlation functions of the relevant observables are determined by homogeneous equations due to Mori-Zwanzig [15].

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(ii) The memory terms included in those resulting equations can be expressed in terms of the mentioned correlation functions of the relevant variables [14,16].
(iii) Using appropriate approximations, especially for the memory kernel, one is able to get solutions of the self-consistent, nonlinear integro-differential equation for the correlation functions which had been done in studying glasses in a series of papers [13,7].

As already stressed the projection formalism can be used in a similar manner to study even the behavior of a single particle in a random environment. In that case only the coordinate of the particle is a relevant observable. Following the line given above for the mode-coupling approach one can derive an equation for the probability distribution function $P(\mathbf{r},t)$ which describes the probability to find a particle at time t in an interval around the point $\mathbf{r}$. Such an equation with a memory term is well known as Nakajima-Zwanzig equation (or generalized master equation) [17]. It can be obtained by applying a suitable projection operator on the total probability distribution in the phase space. Typically, a one-particle distribution function obeys the Fokker-Planck-equation. Recently, using similar arguments as for deriving the Nakajima-Zwanzig equation, a generalized (nonlinear) Fokker-Planck equation has been proposed [6] including a memory term:

$$\partial_t P(\mathbf{r},t) = D\Delta P(\mathbf{r},t) + \nabla \mathbf{F}(\mathbf{r},t)P(\mathbf{r},t) - \lambda \int_0^t P^2(\mathbf{r}-\mathbf{r}',t-t')\partial_{t'}P(\mathbf{r}',t')\mathrm{d}^d r'\mathrm{d}t'. \quad (1)$$

Following [13] the additional last term is originated from the general form of the memory term within the corresponding Nakajima-Zwanzig equation written in the form $\int \hat{K}(\mathbf{r}-\mathbf{r}',t-t')\partial_{t'}P(\mathbf{r}',t')\mathrm{d}^d r'\mathrm{d}t'$. Here, the kernel $\hat{K}$ is expanded in terms of the probability $P(\mathbf{r},t)$. The same arguments as used successfully in the mode-coupling theory [7,8,13,14] lead to a first nonzero contribution when $\hat{K} \simeq P^2$. Thus, we have taken into account the lowest order term in the memory kernel. Higher order terms can also occur but they are irrelevant in the renormalization group approach [6]. In that case where memory effects can be neglected completely ($\lambda = 0$), equation (1) describes the diffusive motion (with diffusion coefficient D) of a particle in an environment defined by the external force field $\mathbf{F}(\mathbf{r},t)$. Physically, such a force field simulates the influence of all other particles of the system. Each particle in a system without any long-range order, such as a glass, can experience locally a different environment. Whereas for $\lambda = 0$ the particle under consideration does not influence its neighborhood the inclusion of the memory term gives rise to a feedback-coupling. Due to that coupling manifested by the memory term in equation (1) the motion of a particle is apparently influenced. The probability to find a certain particle at the point $\mathbf{r}$ at time t is also determined by the probability to find that particle in the surroundings prior the actual observation at t. As pointed out in [6] a positive memory coupling strength ($\lambda > 0$) enhances the probability that a particle is able to visit one of its initially occupied site during a finite time interval. To be more specific, let us consider only the influence of the memory term. In that case equation (1) suggests an increase of the probability $P(\mathbf{r},t)$ in time whenever the particle at $\mathbf{r}'$ to a previous time $t' = t-\tau$ has offered a high tendency to leave this position. In such a manner a positive memory strength favors a return of the particle to a certain point during the sufficient long time interval τ. On the other hand, a negative memory ($\lambda < 0$) should prevent strongly the return to a site initially occupied. As mentioned above, the basic mechanism appears to be very close to so called true self-avoiding walk [3,4]. Within that fundamental model a traveler had been considered who steps randomly however under avoiding sites visited already. The underlying stochastic process for the position $\mathbf{R}(t)$ is determined by a Gaussian distributed noise term and a density $\rho(\mathbf{r},t)$ which varies whenever the walk crosses the point $\mathbf{r}$ at time t. In our model, we study the time evolution for the probability $P(\mathbf{r},t)$ itself. When the factor λ in equation (1) is negative the tracer particle tries indeed to avoid lattice sites which it had been visited already before. Different to the congenial approach [3,4] in our model the avoiding effect is approximated by a non-local feedback term. Moreover, the system depends strongly on the sign of the memory term resulting in a different physical behavior, anomalous diffusion or localization, alternatively. Such a behavior had been observed in more detail applying a dynamical renormalization group approach [6]. An analysis of equation (1) shows the existence of various anomalous diffusion regimes below the critical dimension $d_c = 2$. The results are based on a one loop-expansion and furthermore they are only valid in the vicinity of the fixed point. It is the aim of the present paper to analyze numerically the model introduced above. The simulations presented here support the predicted anomalous diffusive behavior. Moreover, the localization expected in case of $\lambda > 0$ is also manifested by the numerics.

To clarify the role of the memory term in equation (1) the following investigations are restricted to irrelevant force fields $\mathbf{F}(\mathbf{r},t)$ realized for instance if the force field is stochastically time-dependent with a correlation function $\langle F_\alpha(\mathbf{q},t)F_\beta(\mathbf{q}',t')\rangle \sim \delta(t-t')\delta(\mathbf{q}-\mathbf{q}')$ or if the force is time independent, but $\mathbf{F}(\mathbf{r})$ is related to a random potential V with short range correlations, *i.e.* $\langle V(\mathbf{q})V(\mathbf{q}')\rangle \sim \delta(\mathbf{q}-\mathbf{q}')$. In all those cases the renormalization group approach yields asymptotically a superdiffusive regime for a negative feedback-coupling strength where the mean square displacement behaves as $\langle r^2\rangle \simeq t^{1+d/2}$, d is the dimensionality. As discussed before a positive memory strength supports the localization of the particle in the environment of its starting point.

Subsequently, we present the results of a Monte-Carlo simulation of the feedback-coupling model. The main problem of the simulations consist of finding out an adequate procedure which allows us to include both the positive and the negative memory in an appropriate manner. Finally, a slight modification of the original model is discussed by considering a special exponentially

decaying memory kernel denoted as weak memory. It will be argued that such an extended version reflects some features of tracer diffusion in glasses or supercooled liquids. Especially, the model with a weak memory term is suitable to describe the crossover from a regime dominated by anomalous diffusion at short and intermediate time scales to conventional diffusion for sufficient long times.

2 The model

In this paper we focus our attention to the 1-dimensional case. The situation for a 2-dimensional system, which offers logarithmic corrections, has been analyzed in more detail elsewhere [18]. The motion of the tracer particle is defined by a series of discrete jumps within discrete time intervals. Using $\delta\tau$ as an elementary time step, the finite time scale is given by $t = n\delta\tau$ $(n = 0, 1, 2, ...)$. The diffusion is now realized by jumps between neighbored lattice sites within the discrete time t. Now let us define local connection values b_i characterizing the bonds between the adjacent lattice sites i and $i+1$. The transition rates from i to $i+1$ and from i to $i-1$, respectively, for a particle located at lattice site i are defined by

$$k_{i,i+1} = \frac{b_i}{b_i + b_{i-1}} \qquad \text{and} \qquad k_{i,i-1} = \frac{b_{i-1}}{b_i + b_{i-1}} \cdot \quad (2)$$

Thus, $k_{i,i+1} + k_{i,i-1} = 1$, *i.e.* the total probability for a jump of a particle is always 1. The initial values for each b_i are fixed by $b_i = 1$ for all lattice sites. If the connection values remain unchanged, a simple conventional 1-dimensional random walk is realized by those hopping processes. To include also a memory effect, we introduce a self-induced change of the connection values, which gives rise to the feedback of the particle to its environment. That means, the quantities b_i become now time-dependent. After each time step the local connection values have been redefined using the rules

$$\begin{aligned} &b_i(t+\delta\tau) \neq b_i(t) \text{ if the actual jump crosses} \\ &\qquad\qquad \text{the bond between } i \text{ and } i+1, \\ &b_i(t+\delta\tau) = b_i(t) \text{ if the actual jump crosses} \\ &\qquad\qquad \text{another bond.} \end{aligned} \quad (3)$$

The first rule has to be specified in the following manner: a positive memory is defined by a change $b_i(t+\delta\tau) > b_i(t)$, a negative memory requires $b_i(t+\delta\tau) < b_i(t)$. These time-dependent connection values break the symmetry of the transition rates, *i.e.* the local rates for a jump to the left hand side or to the right hand side may be differ from each other after a sufficient long time. Obviously, a multiple crossing of a bond leads to an accumulation effect which is able to increase (or to decrease) the local connection value considerable, also if $|b_i(t+\delta\tau) - b_i(t)| \ll b_i(t)$. It can be argued, that this accumulation effect supports the generation of a (self-induced) localization (in the case of a positive memory) or of a superdiffusion (negative memory).

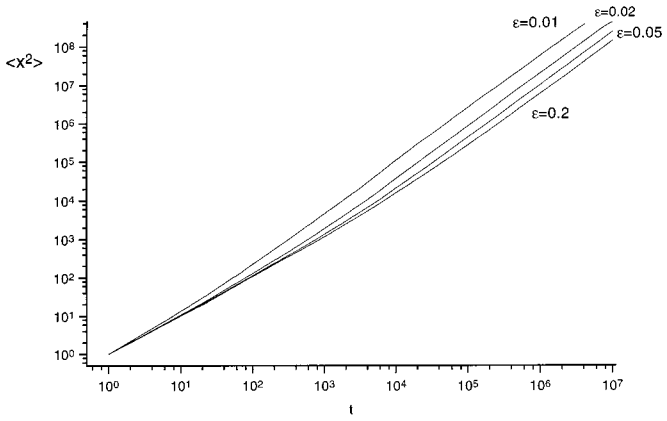

Fig. 1. Mean square displacement for a negative memory with strength $\varepsilon = 0.01$, 0.02, 0.05 and 0.2. The asymptotic behavior for $t \to \infty$ corresponds to a superdiffusion with the universal exponent $2/z = 1.37$.

3 Results

3.1 Superdiffusion

We use the following quantitative rule: each crossing of a bond $(i, i+1)$ by the particle changes the corresponding connection value *via*

$$b_i \to b_i(1-\varepsilon)$$

with $0 < \varepsilon < 1$. Such a relation generates a negative memory. The control parameter ε determines the coupling between particle and environment ($\varepsilon = 0$ corresponds to normal diffusion). We expect that each nonzero ε leads always to a superdiffusive behavior. Thus, the numerical simulations had been realized for various values of ε (see Fig. 1). The determination of the time-dependent mean square displacement shows a normal diffusion for short times and small ε. But after a well defined time $\tau_{\text{cross}}(\varepsilon)$ we obtain a crossover to a superdiffusive behavior

$$\langle x^2 \rangle \sim t^{2/z}$$

with the universal exponent $2/z = 1.37 \pm 0.02$. Let us compare this numerical result with the predictions of the dynamical renormalization group [6]. This calculation taking into account only 1-loop corrections predicts for the exponent $2/z = 3/2$ for $d = 1$, *i.e.* the agreement between numerical simulations and analytical predictions is a reasonable one. Although we are not able to find a unique mapping of our model to that for the true self-avoiding walk [3,4], our exponent is remarkable very close to the exponent 4/3 obtained within that approach. However, it is easy to check that the flow equations for the true self-advoiding walk and the corresponding ones for our model [6] are different.

Let us stress that our previous studies at the critical dimension $d = 2$ are in agreement with the suggestions for the exponent ζ in [4].

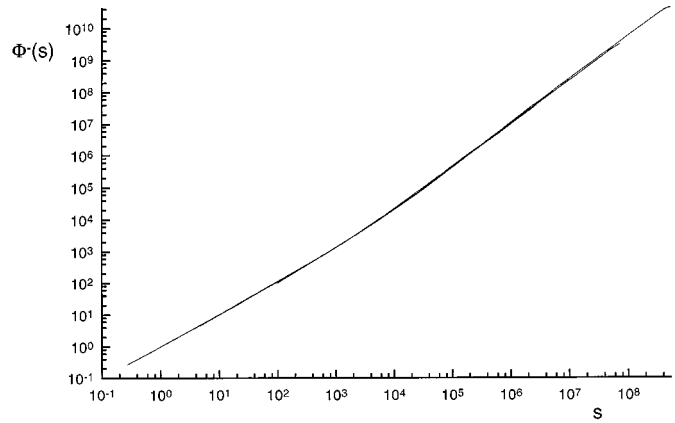

Fig. 2. Master curve of the mean square displacements with negative memory. The collaps of all curves corresponds to universality of the superdiffusion behavior.

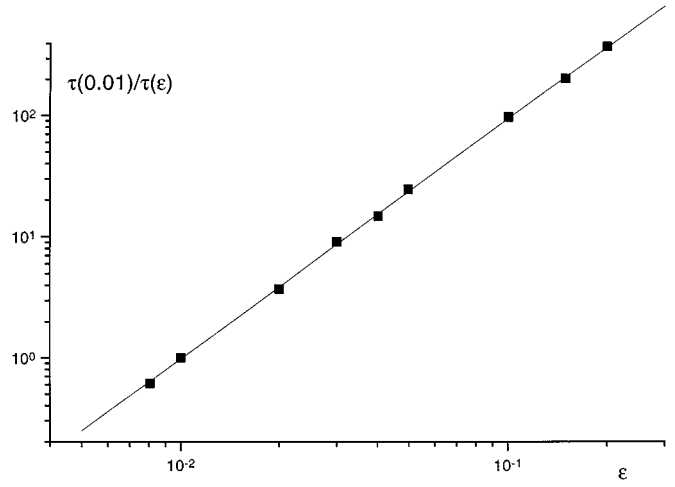

Fig. 3. Inverse crossover time (in units of $1/\tau(0.01)$) as a function of the control parameter ε.

A rescaling of time and coordinates leads to a collapse of all curves presented in Figure 1 onto a scaling function Φ^-, *i.e.* we obtain the general representation

$$\langle x^2 \rangle = \rho\left(\varepsilon\right) \Phi^- \left(\frac{t}{\tau_{\mathrm{cross}}(\varepsilon)} \right)$$

with $\Phi^-\left(s\right) \simeq s$ for $s \to 0$ and $\Phi^-\left(s\right) \simeq s^{2/z}$ for $s \to \infty$, compare Figure 2. The special definition of our model leads immediately to the relation $\rho\left(\varepsilon\right) = \tau_{\mathrm{cross}}(\varepsilon)$. Moreover, Figure 3 shows the crossover time as a function of ε. Obviously, we find the scaling relation

$$\tau_{\mathrm{cross}}(\varepsilon) \sim \varepsilon^{-\theta}$$

with the numerical result $\theta = 1.97 \pm 0.04$.

3.2 Localization

Instead of applying the obvious rule $b_i \to b_i\left(1+\varepsilon\right)$ with $\varepsilon > 0$ numerical arguments suggest to use a weaker additive mapping: each crossing of a bond $(i, i+1)$ by the particle changes the corresponding connection value *via*

$$b_i \to b_i + \vartheta$$

with $\vartheta > 0$. This relation corresponds to a positive memory and we expect for each parameter $\vartheta > 0$ the localization of the particle in a region around the initial position. The determination of the time-dependent mean square displacement shows for short times again a normal diffusion, which decreases continuously after a crossover time $\tau'_{\mathrm{cross}}\left(\vartheta\right)$. Asymptotically, the mean square displacement approaches a constant value. The curves of Figure 4 suggest a localization radius

$$\lim_{t\to\infty} \sqrt{\langle x^2 \rangle} \sim R\left(\vartheta\right).$$

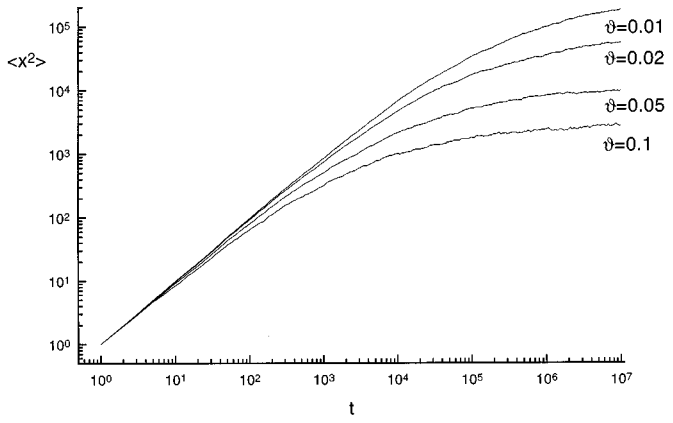

Fig. 4. Mean square displacement for a positive memory (additive mapping) with various strength ϑ.

A rescaling of time and coordinates leads again to a collapse of all curves onto another scaling function Φ^+. The general representation reads

$$\langle x^2 \rangle = R^2\left(\vartheta\right) \Phi^+ \left(\frac{t}{\tau'_{\mathrm{cross}}(\vartheta)} \right)$$

with $\Phi^+\left(s\right) \simeq s$ for $s \to 0$ and $\Phi^+\left(s\right) = 1$ for $s \to \infty$, see also Figure 5. In our model we find the relation $R\left(\vartheta\right) = \sqrt{\tau'_{\mathrm{cross}}(\vartheta)}$. Figure 6 shows $\tau'_{\mathrm{cross}}(\vartheta)$ as a function of ϑ. The numerical results yield

$$\tau'_{\mathrm{cross}}(\vartheta) \sim \vartheta^{-\theta}$$

with $\theta = 2.03 \pm 0.05$. But let us emphasize that, of course, a multiplicative mapping $b_i \to b_i\left(1+\varepsilon\right)$ generates also a localization, depicted in Figure 7. Furthermore, it should be remarked the scaling function Φ^+ is not a universal one, *i.e.* different mapping procedures $b_i(t) \to b_i(t+\delta\tau)$ lead to different functional shapes of the mean square displacement $\langle x^2 \rangle(t)$.

3.3 Probability distribution of the tracer particle

The probability that the particle occupies at the time t the position $x = ja$ (a: lattice unit) is defined as $P(x,t)$.

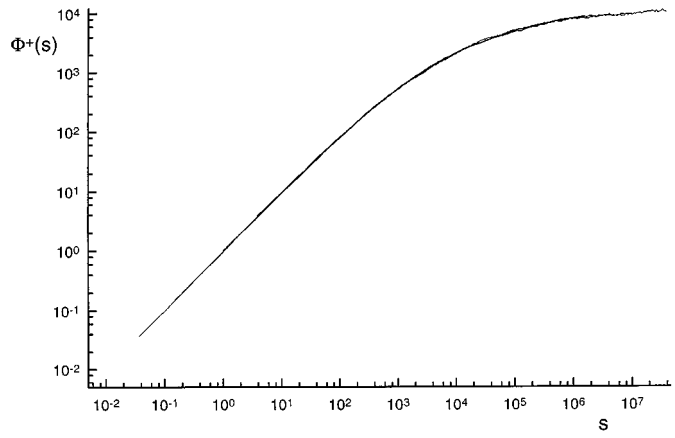

Fig. 5. Master curve of the mean square displacements with positive memory and additive mapping. The collaps of all curves corresponds to universality of the superdiffusion behavior and indicates localization for sufficient long times.

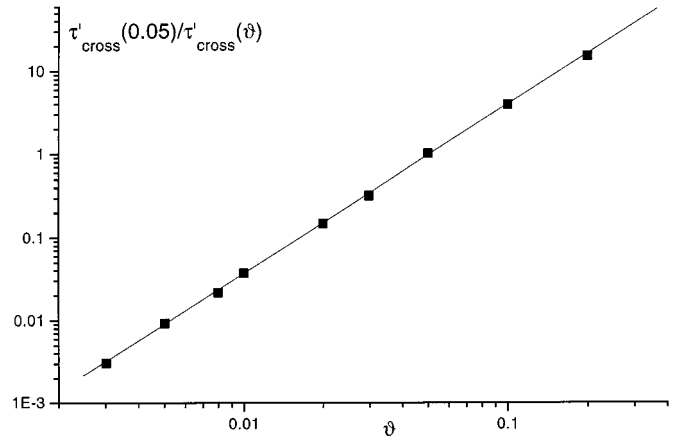

Fig. 6. Inverse crossover time τ' (in units of $1/\tau'(0.05)$) as a function of the control parameter ϑ.

Because of the inversion symmetry we can restrict our investigations onto the probability distribution function $P(|x|,t)$. The knowledge of this function allows the determination of all moments $\langle x^{2n}\rangle$ $(n = 0, 1, 2, ...)$. Figures 8 and 9 show the evolution of $P(|x|,t)$ for the localization case with $\vartheta = 0.01$. It is clear visible, that the probability distribution changes their shape from a Gaussian curve (at very short times) to an exponential like distribution for long times. This transition is continuously, but one can relate only partially the crossover time $\tau'_{\rm cross}(\vartheta)$ with this behavior. Although noticeable deviations from the Gaussian shape occur also for relative short times, we find that they have only a weak influence on the short time behavior of the mean square displacement. But it can be expected that higher moments or combinations of these quantities should indicate the deviations of the probability distribution from the Gaussian shape sooner. The function $P(|x|,t)$ approaches for sufficient long times

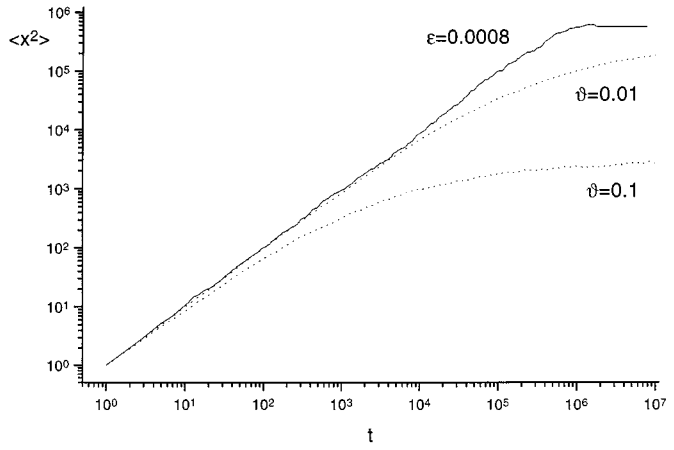

Fig. 7. Comparison of the mean square displacement for a positive memory with multiplicative mapping (full line) and for a positive memory with additive mapping (dotted lines). Both types of mapping show localization.

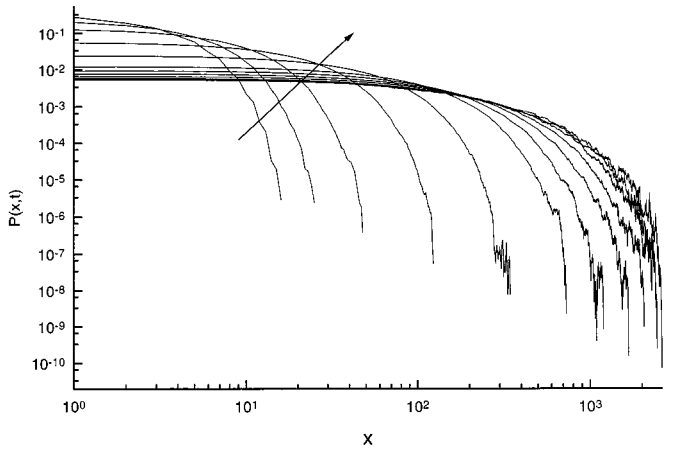

Fig. 8. Evolution of the probability distribution $P(|x|,t)$ (positive memory and additive mapping with $\vartheta = 0.01$) after 19, 44, 142, 1009, 7020, 49 184, 130 414, 345 922, 917 722, 2 434 860, 3 966 045 and 6 460 259 elementary steps. The time increases in the direction of the arrow.

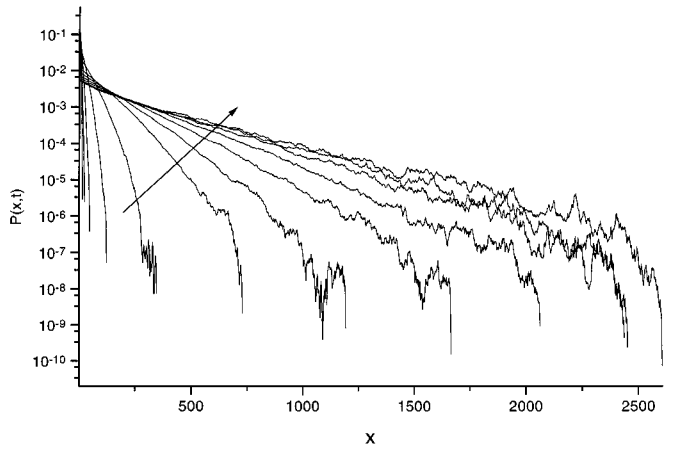

Fig. 9. Half logarithmic representation of the probability distributions $P(|x|,t)$ of Figure 8.

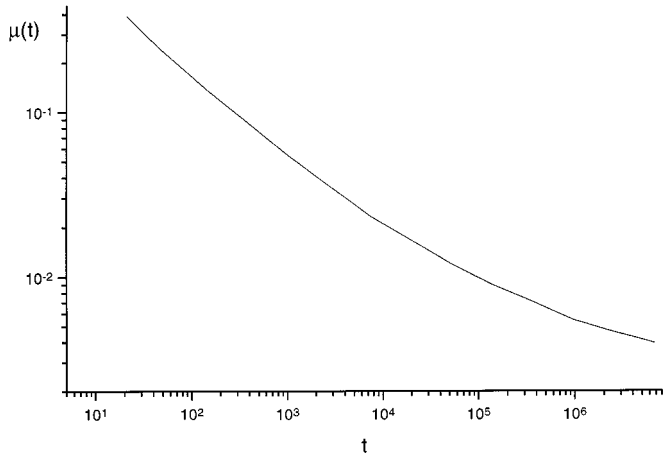

Fig. 10. The function $\mu(t)$ defined in Section 3. with positive memory and $\vartheta = 0.01$).

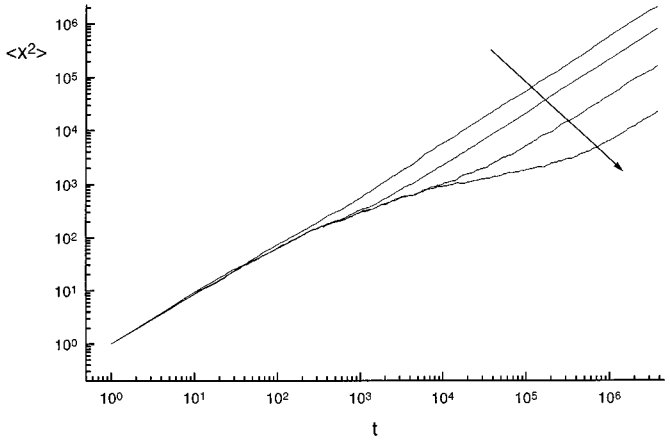

Fig. 11. Mean square displacement as a function of time for a weak positive memory ($\vartheta = 0.1$) with the the control parameter $\zeta = 10^{-2}$, 10^{-3}, 10^{-4} and 10^{-5}. ζ decreases in the direction of the arrow.

to $\exp\{-\mu(t)\,|x|\}$, with $\mu(t) \to$ const. for $t \to \infty$ (see Fig. 10). The half logarithmic representation, compare also Figure 9, reveals that the region nearby to the initial position becomes first of all an exponential-like distribution, whereas the logarithm of the distribution function approaches asymptotically a parabolic shape for large distances, *i.e.* regions far away from the initial point are characterized by the tail of a Gaussian probability distribution. The reason for this behavior can be explained in a simple manner. The particle is able to visit those sites very rarely which are sufficiently far away to the initial point, *i.e.* we expect only small corrections of the corresponding connection values b_i and therefore a nearly Gaussian like behavior of the probability distribution appears. On the other hand, the particle remains frequently in the environment of the initial position. This leads to an accumulation effect, *i.e.* the b_i will be strongly changed and the probability distribution degenerates to an exponential function.

4 Generalization: weak memory

A modification of the rules introduced in equation (3) are introduced as follows. After each time step, the original transformation (3) will be realized. Then, all connection values b_i will be reduced by application of an additional step

$$b_i \to (b_i - 1)\exp\{-\zeta\} + 1. \tag{4}$$

Hence, if the particle crosses not a given bond over a long time interval, the corresponding connection value relaxes to the initial value $b_i = 1$. Equation (4) means that the memory term of the Fokker-Plack equation (1) contains now an additional damping term:

$$\lambda \int_0^t P^2(\mathbf{r} - \mathbf{r}', t - t')\exp\{-\nu(t - t')\}\,\partial_{t'} P(\mathbf{r}', t')\mathrm{d}^d r'\mathrm{d}t' \tag{5}$$

(with $\nu \sim \zeta$). Such an attenuation leads to a shift of the poles originated by the memory term and therefore the critical phenomena indicated for sufficient long time scales $t \gg \nu^{-1} \sim \zeta^{-1}$ do not appear. Instead of that a crossover is expected to a normal diffusion at a characteristic time $\tau^\star \simeq \zeta^{-1}$. This assumption is supported by the numerical results, depicted in Figure 11. For short and intermediate time scales we observe the same behavior as for $\zeta = 0$, *i.e.* firstly the particle shows a normal diffusive behavior followed by the onset of localization. But after a characteristic time $\tau^\star \simeq \zeta^{-1}$ the diffusion becomes again normal. Some features of this behavior are similar to the particle diffusion in real glasses. For example, the cation diffusion in silica glasses (sometime described as a diffusion in quasi 1-dimensional channels [19]) may be influenced by the discussed effects, which should contribute to the well known anomalies of the electrical conductivity in ionic glasses.

A further extension of our model consists of including a power-law damped memory kernel which should give rise to a subdiffusive behavior with an exponent which varies with the exponent of the tail of the feedback term [20].

5 Conclusions

Here, we have presented simulations which strongly support the one-loop renormalization group result [6], after that a positive memory strength below $d_\mathrm{c} = 2$ combined with irrelevant drift forces, compare equation (1), leads surprisingly to a pronounced localization effect of the particle. The result is indeed remarkable, because diffusion under the influence of pure spatially random drift forces [1,2] does not possess localization. Thus, we conclude localization is induced by the memory term exclusively. From that point of view, localization appears for pure dynamical reasons, namely by the feedback-coupling between the particle and the environment which will be observable in case of an arbitrary positive memory

strength below the critical dimensionality. But it can be argued that a strong localization below d_c will also exist above d_c. Such a conclusion is in correspondence with [21] where the existence of a critical λ_c is predicted. Whereas for $d > d_c$ and $\lambda \geq \lambda_c$ the particles are localized, conventional diffusion occurs for $d > d_c$ and $\lambda < \lambda_c$.

On the other hand, a negative memory strength $\lambda < 0$ is related to superdiffusion for $d \leq d_c$. Conventional diffusion is expected to occur above the critical dimension. Although a one dimensional glass system does not exist in nature we believe that some special kinds of glass-formers offering the mixed mobile ion effect [9,10,22] should be considered as possible candidates for that regime.

However, in case that a soft memory term (introduced by Eqs. (4) or (5)) describes the behavior of glassy systems approximatively such anomalous effects are suppressed apparently above a characteristic time scale. We argue that this time scale should be directly related to the typical relaxation time for structural fluctuations known as the α-process in supercooled liquids. Hence, a permanent localization (or superdiffusion) should be realized if this relaxation time diverges. Under that circumstances the glass becomes completely (or sufficiently strong) frozen in the region around the experimentally extrapolated Kauzmann-temperature. The last considerations are in agreement with the results of the conventional mode-coupling theory [13,7,14] for glasses. The theoretical approach predicts a change from liquid-like transport properties to solid-like transport properties with localized particles, at least for a sufficient long time scale. Let us however point out that the conventional mode-coupling theory describes the behavior of collective properties while our research concerns single particles. Moreover, our numerical simulations (and the corresponding renormalization group approach [6]) show both localization and superdiffusion as universal effects determined only by the feedback-coupling. Furthermore, our model is related to the true self-avoiding walk discussed by [3,4]. Although the underlying basic mechanisms between that model and our approach is closely related to each other, there is no apparent mapping of both models. However, our simulations have confirmed the exponent $z = 4/3$ in the cited papers with reasonable accuracy.

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