MEMORY EFFECTS AND DIFFUSION FOR STRONGLY CORRELATED STOCHASTIC SYSTEMS DESCRIBED BY THE GENERALIZED LANGEVIN EQUATION DRIVEN BY A JUMPING PROCESS

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Solutions of the generalized Langevin equation are simulated by using a jumping process as a model of the stochastic force. This force is strongly correlated; we consider two forms of correlations' tail: $\sim 1/t^2$ and $\sim 1/\sqrt{t}$. We demonstrate that remnants of the initial condition can be recognized in the velocity probability distributions after a long time if the correlation function falls slowly. Moreover, the system can exhibit both normal and anomalously slow diffusion which is reflected by the structure of the spectra.

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1. Introduction

The Langevin equation can describe dynamics of the Brownian particle properly if the driving stochastic force is uncorrelated (the white noise) [1]. It is the case only if the correlation time of the fluctuations is much shorter than the time scale of the macroscopic motion. The system reaches the stationary state which is the thermal equilibrium characterized by the temperature T of the heat bath. Quantities describing the system: the temperature, the damping parameter (viscosity) and the particle mass are related to each other due to the fluctuation-dissipation theorem (the Einstein relation).

In many physical problems the correlations of the stochastic force are not negligible. They are encountered in effective descriptions of many-body systems [2,3], in hydrodynamics [4,5], in modeling of transport of the Brownian particles in spatially periodic structures [6], in spectroscopy [7]. In the disordered media long correlations, both in space and time, are often accompanied by the anomalous diffusion [8]. The transport phenomena in dynamical Hamiltonian systems often exhibit anomalous behavior because

(1701)

the corresponding phase space can contain some regular structures [9, 10]. A trajectory sticks to such islands in chaotic environment and abide on regular paths for a long time. The velocity autocorrelation function possesses long tails in this case. An effective stochastic description of such phenomena must be very different from the usual Markovian and Gaussian formalism. Moreover, the Lyapunov exponent equals zero on regular paths which results in much slower memory loss than for the purely chaotic system.

If we require the proper equilibrium state to be achieved in the dynamical evolution, the Langevin equation must be modified. The generalized Langevin equation (GLE), which describes the time evolution of the velocity vector $\boldsymbol{v}(t)$, has then the following form [11]:

$$m \frac{d\boldsymbol{v}(t)}{dt} = -m \int_{0}^{t} K(t-\tau)\boldsymbol{v}(\tau)d\tau + \boldsymbol{F}(t), \qquad (1)$$

where $\mathbf{F}(t)$ is the correlated stochastic force with mean zero and m denotes the particle mass. The memory kernel K(t) describes the generalized viscosity and it is related to the noise autocorrelation function $C(t) = \langle \mathbf{F}(0) \cdot \mathbf{F}(t) \rangle$ via the second fluctuation-dissipation theorem [12]: $K(t) = C(t)/mk_{\rm B}T$, where $k_{\rm B}$ is the Boltzmann constant. Therefore, the equations which correspond to the individual components of the velocity vector are not independent of each other but they are coupled via the scalar product in the autocorrelation function C(t), as the fluctuation-dissipation theorem requires.

The function C(t) defines the driving force F(t) completely only if it has the Gaussian distribution. For strongly correlated processes, however, it is not the case because the central limit theorem does not hold [13]. Therefore, we have to assume a specific model for F(t), by demanding a given form of C(t) and vanishing mean. A convenient possibility is to apply a jumping process $\xi(t)$ which has been introduced in Ref. [14]. This Markovian and stationary process is defined in terms of two probability distributions: the jump-size distribution $Q(\delta \xi = \xi - \xi')$ and the waiting time distribution $P_{\rm P}(\tau)$. It possesses a slowly decaying autocorrelation function.

The motion of the Brownian particle, described by the GLE (1), must reflect fluctuation properties of the driving force $\mathbf{F}(t) = \boldsymbol{\xi}(t)$ and the shape of the autocorrelation function is an important quantity which influences the time the system needs to reach its equilibrium state. Moreover, one can expect that the memory about initial conditions are preserved for a long time if the noise is strongly correlated. Therefore, the GLE could be used as a realistic and convenient description of systems far from equilibrium. In this paper we analyze the above problems in details. In Sec. 2 we present the model of the noise and general properties of the GLE. In Sec. 3 we discuss the quantities which are responsible for the speed the memory about the initial conditions is lost. Moreover, we analyze transport properties of the system and demonstrate that they are related to the memory effects. In Sec. 3 the GLE is solved for two specific forms of the stochastic force.

2. Model of the noise and its application to the GLE

The jumping process is defined as a two-dimensional vector $\boldsymbol{\xi}$. For the jump-size distribution Q we assume the Gaussian form. Subsequently, we assume that $\boldsymbol{\xi}$ has the unitary length: $\boldsymbol{\xi}(t) = (\xi_1 = \cos(\phi), \xi_2 = \sin(\phi))$ [14]. Therefore, the distribution Q becomes:

$$Q(\delta \boldsymbol{\xi}) \sim e^{-(\boldsymbol{\xi} - \boldsymbol{\xi}')^2 / 2\sigma^2} \sim e^{\cos(\phi - \phi') / \sigma^2}, \qquad (2)$$

where σ is a given width. The waiting time distribution $P_{\rm P}(\tau)$ is Poissonian:

$$P_{\rm P}(\tau) = \nu(\boldsymbol{\xi}) e^{-\nu(\boldsymbol{\xi})\tau} , \qquad (3)$$

and it determines the size of intervals of constant process value. The jumping rate $\nu(\boldsymbol{\xi})$ depends on the process value and, therefore, $\boldsymbol{\xi}(t)$ can be regarded as a generalization of the well-known kangaroo process [15,16]. This function is assumed in the following form:

$$\nu(\phi) = \frac{4}{1-\alpha} \frac{|\sin(\phi)|^{\alpha}}{|\cos(\phi)|}, \qquad (4)$$

where $0 < \alpha < 1$. The process $\boldsymbol{\xi}(t)$, defined by means of Eqs. (2)–(4) possesses the autocorrelation function which can be approximated by the following integral

$$C(t) = 4 \int_{0}^{\pi/2} \frac{e^{-\nu(\phi)t}}{\nu(\phi)} \, d\phi \,.$$
(5)

Its tail has the power-law shape for ν given by Eq. (4):

$$\mathcal{C}(t) \sim t^{1-1/\alpha}, \quad \text{for} \quad t \to \infty.$$
 (6)

Therefore, the process $\boldsymbol{\xi}(t)$ constitutes a 1/f noise.

The GLE (1) can be solved by using Laplace transforms. As a result, we obtain the following expression for the stochastic trajectory:

$$\boldsymbol{v}(t) = R(t)\boldsymbol{v}(0) + m^{-1} \int_{0}^{t} R(t-\tau) \boldsymbol{F}(\tau) d\tau , \qquad (7)$$

A. KAMIŃSKA, T. SROKOWSKI

where the Laplace transform of the resolvent R(t) is given by the equation

$$\widetilde{R}(s) = \frac{1}{s + \widetilde{K}(s)}.$$
(8)

From Eq. (7) we conclude that the resolvent R(t) is directly related to the velocity autocorrelation function

$$C_{v}(t) = \langle \boldsymbol{v}(0)\boldsymbol{v}(t)\rangle = \frac{k_{\rm B}T}{m}R(t).$$
(9)

To obtain the above relation, one multiplies the Eq. (7) by $\boldsymbol{v}(0)$ and takes the average over the statistical ensemble. Applying the step-wise jumping process $\boldsymbol{\xi}(t)$ as a model of the force $\boldsymbol{F}(t)$, one can reduce the above equation to a sum over consecutive jumps which take place at times t_i : $t_0 = 0, \ldots, t_n = t$, and correspond to the process values $\boldsymbol{\xi}_i$:

$$\boldsymbol{v}(t) = R(t)\boldsymbol{v}(0) + m^{-1} \left[\boldsymbol{\xi}_{n+1} \int_{0}^{t-t_n} R(\tau) \, d\tau + \sum_{k=1}^n \boldsymbol{\xi}_k \int_{t-t_k}^{t-t_{k-1}} R(\tau) \, d\tau \right] \,. \tag{10}$$

3. Memory about the initial condition and anomalous diffusion

In the absence of a conservative force, the velocity distribution of the Brownian particle changes its shape due to the subsequent jumps of the random driving. Then if there is a small number of jumps, the shape of the initial distribution survives for a long time. The probability that memory about the initial conditions is not lost depends on the jumping process autocorrelation function. The existence of long tails of C(t) implies that after a long time there are still some trajectories in the statistical ensemble for which no jump has yet occurred. More precisely, the conditional probability that the value of the jumping process $\boldsymbol{\xi}(t)$ is kept constant during the time t (no jump takes place) is $e^{-\nu(\boldsymbol{\xi})t}$, according to Eq. (3). The Eq. (4) implies in turn that this time can be extremely long for $\phi \approx 0$. We can obtain the full probability that no jump occurs up to the time t by taking into account all process values $\boldsymbol{\xi}$:

$$P_{nj}(t) = \int_{0}^{2\pi} e^{-\nu(\boldsymbol{\xi})t} P(\phi) d\phi \sim \mathcal{C}(t) , \qquad (11)$$

where we have assumed that the system is in its stationary state $P(\phi) = 1/\nu$ [14]. Therefore, the longer tails of the jumping process autocorrelation function, the smaller jump probability.

1704

Let us now consider the solutions of GLE, driven by the jumping process, on the assumption that the jumping probability is small. In this limit no jump occurs and the velocity components are given by the following simple expressions:

$$v_x(t) = m^{-1}\xi_1 \mathcal{D}_t(t), \qquad v_y(t) = m^{-1}\xi_2 \mathcal{D}_t(t),$$
 (12)

where $\mathcal{D}_t(t) = \int_0^t R(\tau) d\tau$ and the initial condition is assumed as $\boldsymbol{v}(0) = 0$. We want to find the Brownian particle velocity probability distribution $p(\boldsymbol{v}, t)$, knowing the stationary distribution of the jumping process $P(\phi) = 1/\nu(\phi)$. For the distribution of both components of the jumping process, ξ_1 and ξ_2 , we obtain:

$$P_{1}(\xi_{1}) = \sum_{\{\phi: \xi_{1} = \cos\phi\}} \frac{1}{\nu(\phi)|\cos'(\phi)|} = \frac{1-\alpha}{2} \frac{|\xi_{1}|}{(1-\xi_{1}^{2})^{(1+\alpha)/2}},$$

$$P_{2}(\xi_{2}) = \sum_{\{\phi: \xi_{2} = \sin\phi\}} \frac{1}{\nu(\phi)|\sin'(\phi)|} = \frac{1-\alpha}{2} \frac{1}{|\xi_{2}|^{\alpha}},$$
(13)

for $|\xi_{1,2}| \leq 1$ and zero elsewhere. Therefore, the required relation between both probability distributions is given by a simple variable transformation:

$$p(v_x, t) = m \frac{P_1(mv_x/\mathcal{D}_t(t))}{\mathcal{D}_t(t)},$$

$$p(v_y, t) = m \frac{P_2(mv_y/\mathcal{D}_t(t))}{\mathcal{D}_t(t)}.$$
(14)

From the Eq. (14) some general conclusions about the distribution p(v, t)can be inferred. Since the distribution $P_1(\xi_1)$ is infinite at $\xi_1 = \pm 1$, the distribution of the first velocity component must possess two peaks positioned at $v_x = \pm \mathcal{D}_t/m$ which result from splitting of the initial peak $p(v_x, 0) = \delta(v_x)$. They can either approach each other or go outwards with time; the movement is governed by the function R(t). The jumps actually destroy the peaks. The time-dependence of their relative height is proportional to the probability that no jump has occurred, which is given by Eq. (11). The distribution of the second velocity component is different because P_2 has only one singularity. Therefore, $p(v_y, t)$ possesses a single peak at $v_y = 0$ as a remnant of the initial condition whose height decreases gradually with time.

Knowing the GLE solution, we can evaluate the Brownian particle position from the equation $\dot{\boldsymbol{r}} = \boldsymbol{v}$ which allows us to determine the diffusion properties of the system, in particular the diffusion coefficient \mathcal{D} , by taking the limit of infinite time. The mean square displacement of the Brownian particle is related to the velocity autocorrelation function due to the Green–Kubo identity [17]:

$$\langle \boldsymbol{r}^2(t) \rangle = \int_0^t (t-\tau) \mathcal{C}_v(\tau) d\tau \,. \tag{15}$$

Using Eq. (9), we obtain the following expression for the diffusion coefficient:

$$\mathcal{D} = \lim_{t \to \infty} \frac{\langle \mathbf{r}^2(t) \rangle}{2t} = \frac{k_{\rm B}T}{m} \lim_{t \to \infty} \int_0^t R(t) dt = \frac{k_{\rm B}T}{m} \lim_{t \to \infty} \mathcal{D}_t(t) \,, \qquad (16)$$

The above equation establishes a relation between the transport properties of the system (the diffusion coefficient) and the movement of peaks in the distribution $p(v_x, t)$ which is determined by the function $\mathcal{D}_t(t)$. On the other hand, the resolvent R(t) is related to the noise autocorrelation function $\mathcal{C}(t)$, due to the Eq. (8) and the fluctuation-dissipation theorem. Defining the characteristic correlation time $\tau_{\rm cor} = \int_0^\infty \mathcal{C}(t) dt$ and taking into account that $\tau_{\rm cor} = \widetilde{\mathcal{C}}(s = 0)$ and $\mathcal{D} = \widetilde{\mathcal{C}}_v(s = 0)$, we can distinguish three cases.

(1) $\mathcal{D} < \infty$ and $\mathcal{D} \neq 0$ (the normal diffusion). $\tau_{\rm cor}$ is then finite. For the algebraic tails of $\mathcal{C}(t)$, $\sim 1/t^p$, this case corresponds to the condition p > 1. Since $\widetilde{R}(s=0)$ is finite as well, the Brownian particle diffusion is normal. The peaks in the $p(v_x, t)$ distribution tend to fixed positions: $v_x = \pm \mathcal{D}/m$.

(2) $\mathcal{D} = 0$ (the subdiffusion). The noise autocorrelation function $\mathcal{C}(t)$ falls slowly with time and then $\tau_{\rm cor}$ diverges. The motion is subdiffusive in this case. The peaks in the $p(v_x, t)$ distribution shift initially outwards but finally they return to the origin.

(3) $\mathcal{D} = \infty$ (the superdiffusion). The condition $\tau_{\rm cor} = 0$ can be satisfied only if $\mathcal{C}(t)$ is negative on some interval. It cannot happen for the jumping process discussed in this paper (see Eq. (5)).

4. Numerical examples

The probability distributions and moments for specific cases can be calculated by means of the Monte Carlo method by using the Eq. (10). We assume such form of the noise autocorrelation function C(t) which falls algebraically with time in the asymptotic regime and is given by Eq. (5). This equation reproduces accurately the jumping process autocorrelation function if the width σ in Eq. (2) is sufficiently large. In the following, we solve the GLE using the stochastic force defined by the Eq. (4) with two values of α : 1/3 and 2/3. In all numerical calculations we assume $k_{\rm B} = m = T = 1$.

1706

4.1.
$$\alpha = 1/3$$

According to Eq. (6), the tail of the autocorrelation function of the jumping process for $\alpha = 1/3$ falls like t^{-2} . For the sake of simulations of the GLE solutions, it is necessary to have an analytic expression which accurately approximates the process autocorrelation function for all times. This expression is the following

$$C(t) = \frac{1 - 6t \exp(-6t) - \exp(-6t)}{18t^2}.$$
(17)

Fig. 1 presents a comparison of the above formula with the exact shape of C(t); the agreement appears quite good for all times. The exact C(t) has been obtained from the numerical simulations of individual trajectories $\boldsymbol{\xi}(t)$, according to probability distributions Q and $P_{\rm P}$; from now on, we assume in numerical calculations $\sigma = 2.5$. Those trajectories constitute the statistical ensemble over which the expression $\boldsymbol{\xi}(0)\boldsymbol{\xi}(t)$ is averaged. Moreover, the formula (17) possesses a simple Laplace transform: $\tilde{C}(s) = 1/3 - s \ln(1 + 6/s)/18$. Therefore, the Laplace transform of the resolvent of the GLE takes the form:

$$\widetilde{R}(s) = \frac{1}{s + 1/3 - s\ln(1 + 6/s)/18}.$$
(18)

The above equation allows us to determine the diffusion properties of the system already at this stage of the analysis. We obtain: $\tau_{\rm cor} = 1/3$ and $\mathcal{D} = \tilde{C}_v(s=0) = 3k_{\rm B}T/m$. Therefore, the diffusion is normal.



Fig. 1. The autocorrelation function C(t) for the case $\alpha = 1/3$ obtained from the trajectory simulations with $\sigma = 2.5$ (solid line) and calculated from Eq. (17) (dashed line).

The inversion of the transform (18) can be performed by the usual method, namely by the derivation of the integral along the straight line parallel to the imaginary axis. The integration area involves two simple poles and a cut between two branching points: -6 and 0. We get the following result:

$$R(t) = e^{-at} \left(c_1 \sin bt + c_2 \cos bt \right) - 18 \int_0^6 \frac{x e^{-tx} \, dx}{\left[18x - x \, \ln(6/x - 1) - 6 \right]^2 + x^2 \pi^2} \,, \tag{19}$$

where the constants a = 0.3778, b = 0.0725, $c_1 = 0.3813$ and $c_2 = 2.1288$, which represent the position of poles in Eq. (18), have been obtained numerically. The expression (19) can be approximated in the limit of large times. The first term can be neglected; the evaluation of the integral is simplified because in the asymptotic regime only small values of the integration variable count. Finally we get $R(t) = 1/2t^2$ for $t \to \infty$. Therefore, the tail of the velocity autocorrelation function $C_v(t)$ has the same time dependence as that of C(t).

Having the resolvent R(t) calculated, we can determine the Brownian particle velocity from trajectory simulations, using the Eq. (10), and construct the probability density distribution p(v,t). We assume the initial condition v(0) = 0. Fig. 2 presents $p(v_x, t)$ for short times obtained both from the simulations and from Eq. (14). The marked agreement confirms that at such short time the jump probability is very small and the motion is



Fig. 2. The velocity distribution $p(v_x, t)$ for the case $\alpha = 1/3$ obtained both from the simulations (solid line) and from Eq. (14). The narrow distribution corresponds to t = 0.1 and the wide one to t = 0.3.

predominantly deterministic. Since near the point t = 0 $R(t) \approx 1$, the peaks are positioned at $v_x \approx \pm t$ and they move outwards because R(t) is positive $(\mathcal{D}_t(t) \text{ rises})$. This behavior changes for larger times because R(t) becomes negative; the peaks turn back to the origin and stop at $v_x = \pm \mathcal{D} = \pm 3$. The gradual transition of the distribution shape to the equilibrium, for slightly larger times, is presented in Fig. 3. The movement of peaks in $p(v_x, t)$ for large times is illustrated in Fig. 4. If time exceeds the value t = 15, the height of the peaks becomes very small and their backward motion towards the points $v_x = \pm 3$ is not visible. That relatively fast memory loss results from the rapid decay of $\mathcal{C}(t)$.



Fig. 3. The time evolution of the velocity distribution $p(v_x, t)$ for the case $\alpha = 1/3$.



Fig. 4. The same as in Fig. 3 but for larger times.

4.2.
$$\alpha = 2/3$$

The integral (5) has the tail which falls like $1/\sqrt{t}$ for $\alpha = 2/3$. The resolvent R(t) for C(t) in this form can be derived relatively easily and it is very simple [18]. However, at small times the Eq. (5) has a very different shape and assumes a finite value. Then the function $1/\sqrt{t}$ cannot be used to evaluate the resolvent. Instead, we apply the following function

$$\mathcal{C}(t) = \frac{\pi\sqrt{3}\operatorname{erf}(\sqrt{12t})}{12\sqrt{t}},\qquad(20)$$

where $\operatorname{erf}(x)$ stands for the error function. The above expression perfectly reproduces the shape of the exact jumping process autocorrelation function for all times. Unfortunately, the Laplace transform of the above expression is not an elementary function and attempts to find R(t) similarly as in the preceded subsection are neither effective nor expedient. Instead, we determine the function R(t) directly from $\mathcal{C}(t)$ as the numerical solution of the equation

$$\frac{dR(t)}{dt} = -\int_{0}^{t} K(t-\tau)R(\tau)d\tau, \qquad (21)$$

which has been obtained by inversion of the Laplace transform in the Eq. (8) and by taking into account that R(0) = 1. The Volterra integro-differential equation (21) possesses the kernel which depends on the difference of its arguments (the convolution equation). That property suggests a method of solution. We approximate the equation by applying the second order central finite difference scheme, namely the Euler method [19], for the differential



Fig. 5. The function R(t) for the case $\alpha = 2/3$ obtained from Eq. (21).

1710

component of the equation and the trapezoid rule for its integral part [20]. The letter method is a kind of quadrature formulas which are often used for the numerical evaluation of integrals. The function R(t), obtained numerically from Eq. (21), has been presented in Fig. 5. It has an oscillatory pattern: the curve fluctuates around R(t) = 0 and the oscillations die down very slowly.

We get the velocity probability distributions $p(\boldsymbol{v},t)$ by solving Eq. (21) simultaneously with the integrals in the Eq. (10). The distributions of the first component are presented in Fig. 6. The times have been so chosen to illustrate the intricate behavior of the peaks corresponding to the initial



Fig. 6. The time evolution of the velocity distribution $p(v_x, t)$ for the case $\alpha = 2/3$.

condition $p(v_x, 0) = \delta(v_x)$: initially they go inwards, then — outwards. Obviously, this movement reflects the oscillatory structure of the function R(t). Finally, in the limit of infinite time, the peaks must converge back to the origin because $\tau_{\rm cor} = \infty$ and then, according to Eq. (8), $\mathcal{D} = \tilde{R}(s = 0) = 0$. This result also means that the Brownian particle motion is subdiffusive. A striking feature of the distributions presented in Fig. 6 is a substantial height of the peaks which hardly diminishes with time. Such a strong manifestation of memory about the initial condition is a direct result of the slow decay of the function $\mathcal{C}(t)$ and, consequently, of the slow increase of the jump probability, according to the Eq. (11).

Fig. 7 shows probability distributions for the component v_y . As expected, there is only one peak, positioned at the origin, which dwindles slowly with time.



Fig. 7. The time evolution of the velocity distribution $p(v_u, t)$ for the case $\alpha = 1/3$.

In Ref. [14] the probability distributions of both velocity components for the case $\alpha = 1/2$ has been presented. Qualitatively, this case is similar to that discussed above: the diffusion is also anomalously weak and the peaks in the $p(v_x, t)$ distribution tend to the origin in the limit of large time.

5. Conclusions

The jumping processes can be used as models of correlated stochastic forces in the GLE. Then this equation can be solved by means of the stochastic trajectory simulations in the framework of the Monte Carlo methods. The model used in this paper was designed for non-Gaussian processes possessing power-law tails of the driving force autocorrelation function C(t). This function enters the presented formalism in two ways: it characterizes the jumping process the values of which are sampled along the stochastic trajectory by means of the Monte Carlo method and, on the other hand, its approximate form directly determines the resolvent R. Therefore, the results of the simulations can be consistent with the fluctuation-dissipation theorem only if the form of C(t) inserted into Eq. (8) is a good approximation of that of the jumping process for all times, not only for the tails.

We have shown that the stochastic system described by the GLE preserves the memory about its initial condition for a long time which depends on how fast the function C(t) falls. The calculated spectra exhibit the peaks (the remnants of the initial condition) which are especially pronounced for the case $\alpha = 2/3$, *i.e.* for very slowly decaying $C(t) \sim 1/\sqrt{t}$ $(t \to \infty)$. Moreover, there is a direct connection between the noise autocorrelation function C(t) and the transport properties of the system. The infinite correlation time $\tau_{\rm cor}$ results in the anomalously slow diffusion. The movement of peaks in the velocity distribution, which correspond to the initial condition, is governed by the resolvent R and the points they tend to are given by the diffusion coefficient.

The memory effects discussed in this paper trace back to the waiting time distribution of the consecutive jumps which is Poissonian. However, since it depends on the process value $\boldsymbol{\xi}$, the intervals of constant $\boldsymbol{\xi}$ can be very long for the long-time correlations and render that the probability that no jump has yet happened is considerable even after relatively long time. Those long intervals are the source of both long correlation tails of the jumping process and the memory effects in the GLE solutions. Another consequence of the existence of long tails in the distributions is weakening of the diffusion process. A similar phenomenon is observed in the framework of the continuous time random walk [21]. In that approach, the trapping of the Brownian particle, which results in the subdiffusion, comes from the power-law waiting time distribution.

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