A Paradox in the Langevin Equation with Long-Time Noise Correlations

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Abstract

We solve the generalized Langevin equation driven by a stochastic force with power-law autocorrelation function. A stationary Markov process has been applied as a model of the noise. However, the resulting velocity variance does not stabilizes but diminishes with time. It is shown that algebraic distributions can induce such non-stationary affects. Results are compared to those obtained with a deterministic random force. Consequences for the diffusion process are also discussed.

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Modeling a physical system in terms of Langevin formalism must take into account the nature and origin of the stochastic force. Usually that force is taken in the form of the white noise but in many cases that is an unrealistic idealization. Among the systems possessing a finite noise correlation time, those with power-law (algebraic) correlations are especially interesting because of lack of characteristic time scale and divergent moments. Such systems are not unusual. The algebraic random force autocorrelation function (FAF) appears in the fluid dynamics and linearized hydrodynamics. For such phenomena as the noise-induced Stark broadening and nuclear collisions, correlation functions proportional to $1/t$ have been found. The latest form of correlations is of special importance for molecular dynamics because it corresponds to the problem of scattering inside a periodic lattice.

For systems with finite noise correlation time, the ordinary Langevin equation must be generalized to ensure proper fluctuation-dissipation relations. In the absence of external potential, this equation has the form

$$m \frac{dv(t)}{dt} = -m \int_0^t K(t-\tau)v(\tau)d\tau + F(t)$$

(1)

where $F(t)$ is a stochastic force and $K(t)$ denotes the retarded friction kernel. The fluctuation-dissipation theorem imposes the relation: $K(t) = \langle F(0)F(t) \rangle/mT$, with temperature $T$ and mass $m$. We require $\langle F(t) \rangle = 0$ and the following FAF:

$$C_F(t) \equiv \langle F(0)F(t) \rangle = \begin{cases} \beta T/\epsilon & \text{for } t \leq \epsilon \\ \beta T/t & \text{for } t > \epsilon \end{cases}$$

(2)

where $\epsilon$ is a small number. The coefficient $\beta$ we set equal to one. The solution of Eq.(1) with the initial condition $v(0) = 0$ takes the form

$$v(t) = g(t) + \int_0^t R(t-\tau)g(\tau)d\tau$$

(3)

where $g(t) = m^{-1}\int_0^t F(\tau)d\tau$ and the resolvent is given by $R(t) = \exp(-at)(c_1 \sin bt + c_2 \cos bt)+m \int_0^\infty x\exp(-tx)/[(mx+E_1(\epsilon x)-1)^2+\pi^2]d\tau$. The modified integral exponential function $E_1(x)$ is defined by the series: $E_1(x) = \gamma + \ln x + \sum_{n=1}^{\infty} x^n/n!n$, where $\gamma = 0.5772157\ldots$ is the Euler constant. The other constants are fixed in the following at the values: $a = -3.52832$, $c_1 = -4.76673$, $c_2 = -5.35498$ and $b = 2.49975$, corresponding to $\epsilon = 0.01$ and $m = 1$.

We are interested in evaluation of the second moment of velocity distribution $\langle v^2(t) \rangle$. It can be obtained directly from (3):

$$\langle v^2(t) \rangle = 2\int_0^t d\tau(t-\tau)C_F(\tau) + 2\int_0^t d\tau \int_0^\tau ds_1 \int_0^\tau ds_2 R(t-\tau)C_F(|s_1-s_2|)$$

$$+ \int_0^\tau d\tau \int_0^\tau ds \int_0^\tau ds_1 \int_0^\tau ds_2 R(t-\tau)R(t-s)C_F(|s_1-s_2|).$$

(4)

Some of the above integrals have to be performed numerically. The result for $T = 1$ is presented in Fig.1. As expected, the system reaches the equilibrium state.

In the following, we will refer to the above result as "analytical". Alternatively, we can introduce a concrete stochastic process characterized by covariance in the form (2) and calculate $\langle v^2 \rangle$ from a Monte Carlo simulation. We apply the "kangaroo process" (KP). It is defined as a stepwise random function: $F(t) = F_i = \text{const}$ in the time interval

\[\text{[Continued on next page]}\]
also the KP covariance \([10,11]\) \(C_{KP}\) can be expressed in terms of the distribution \(P(s)\)

\[
C_{KP}(t) = 3\eta^{-1/3} \int_{\eta}^{\infty} s^{-2/3} \exp(-t/s) P(s)ds.
\]

Inserting \(F(t)\) into Eq. (3) allows us to determine the velocity time series of the Brownian particle. The variance at a given time \(t\) is obtained simply by calculating \(v(t)\), squaring it and averaging over many trajectories. Fig.1 presents the result: \(\langle v^2 \rangle\) does not stabilize at the expected value \(\langle v^2 \rangle = T/m\) but instead it dwindles with time, obeying the approximate relation \(\langle v^2 \rangle(t) \sim t^{-0.67}\).

The above outcome is surprising because the stationary process brings about an apparently non-stationary result. Moreover, according to (4), \(\langle v^2 \rangle\) is completely determined by the covariance of \(F\) and every simulation satisfying (2) should reproduce the analytical result. In order to understand the origin of that inconsistency, let us reconsider in details how actually the stochastic force value enters the Langevin equation. Evaluation of the Brownian particle velocity requires the value of \(F\); its actual non-stationary result. Moreover, according to (4), \(\langle v^2 \rangle\) is completely determined by the covariance of \(F\) and every simulation satisfying (2) should reproduce the analytical result. In order to understand the origin of that inconsistency, let us reconsider in details how actually the stochastic force value enters the Langevin equation. Evaluation of the Brownian particle velocity requires the value of \(F\) at a given time \(t\). For that purpose the distribution of \(s\) is crucial because this value follows from the length of current interval in the stepwise evolution of KP. However, the requirement that we choose only those intervals which contain the time \(t\) imposes some bias, e.g. longer intervals are more probable. Therefore a distribution we actually use in the Langevin equation (the "effective" interval distribution), may not be identical with \(P(s)\). Its cumulative distribution function, \(\Phi(s,t)\), can be derived in the following way. First let us consider \(s \leq t\) and assume that \(t\) is found in \(n+1\) interval, i.e. \(S_n = s_1 + s_2 + \ldots + s_n < t\) and \(S_{n+1} > t\). The probability that the sum of \(n\) intervals yields a value between \(x\) and \(x+dx\) we denote by \(P_n(x)dx\), providing that each component has the distribution \(P(s)\). The distribution function \(\Phi(s,t)\) is just equal to the conditional probability that an interval is larger than \(t-x\), for any \(x\) between \(t-s\) and \(t\), and any \(n\) from 1 to \(N\), where \(N\) denotes the integer part of \(t/\eta\): \(\Phi(s,t) = \sum_{n=1}^{N} \int_{s_n}^{t} \int_{t-x}^{t} P(x)dx P(x)dx\). Introducing \(S(x) = \sum_{n=1}^{N} S_n(x)\) and inserting \(P(x)\) from (3), we get the following equation:

\[
\Phi(s,t) = \eta^{1/3} \int_{t-s}^{t} S(x) [(t-x)^{-1/3} - s^{-1/3}]dx \quad \text{for} \quad \eta \leq s \leq t.
\]
For $s > t$ the lower limit of integration extends to zero. Moreover, we have to take into account also events for which $t$ is contained already in the first interval. The final formula reads:

$$\Phi(s, t) = \frac{1}{3} \left\{ \int_0^t S(x)[(t - x)^{-1/3} - s^{-1/3}]dx + t^{-1/3} - s^{-1/3} \right\} \quad \text{for} \quad s > t. \quad (9)$$

The direct evaluation of $S(x)$ is very difficult. We can avoid it utilizing the normalization condition $\Phi(\infty, t) = 1$. The function $S(x)$ must then satisfy the integral equation

$$\int_0^t S(x)(t - x)^{-1/3}dx + t^{-1/3} = \eta^{-1/3} \quad \text{for} \quad s > t. \quad (10)$$

called Abel’s equation. It possesses a weakly singular kernel, depending only on the difference of its arguments. Therefore we can apply the Laplace transforms technique to solve it \cite{12}. The solution is of the form

$$S(x) = c_T \eta^{-1/3} x^{-2/3} - \delta(x), \quad (11)$$

where a constant $c_T = 1/\left[\Gamma(1/3)\Gamma(2/3)\right] \approx 0.2757 \ldots$ contains the Gamma function. Inserting $S(x)$ to (8) and (9) and evaluating integrals gives us the expression for $\Phi(s, t)$. To obtain the probability distribution $\mathcal{P}(s, t)$, we have to differentiate $\Phi(s, t)$ over $s$. The final result is simple:

$$\mathcal{P}(s, t) = \begin{cases} c_T [t^{1/3} - (t - s)^{1/3}] s^{-4/3} & \text{for} \quad \eta \leq s \leq t \\ (c_T t^{1/3} + \eta^{1/3}/3) s^{-4/3} & \text{for} \quad s > t. \end{cases} \quad (12)$$

The effective interval distribution appears to be time-dependent and consisting of two branches which do not join smoothly. We encounter a similar problem asking about the mean time we must wait for a bus, providing we know the average time interval between subsequent bus arrivals ($\tau$). The answer is not $\tau/2$, as one could expect, but just $\tau$. This "waiting-time paradox" \cite{13} can be elucidated by calculating the effective, time-dependent probability distribution, analogous to (12). In that case, however, the original distribution is an exponential which results in the fast equilibration and the effective distribution asymptotically becomes time-independent. For $\mathcal{P}(s, t)$ it never happens. Moreover, since the probability $\mathcal{P}(s > t, t) = \int_t^\infty \mathcal{P}(s, t)ds = 3c_T \approx 0.83$ does not diminish with time but remains constant, the entire distribution shifts with time towards long intervals. In fact, this outcome is not unexpected because all moments of $\mathcal{P}(s, t)$, as well as of $P(s)$, are divergent. On the other hand, long intervals correspond to small values of the process itself, which points out a reason of declining of the variance. To derive expression for the effective variance $\mathcal{V}(t)$, we can use Eq.(3) substituting $\mathcal{P}(s, t)$ for $P(s)$. Evaluation of the integral gives us the final formula

$$\mathcal{V}(t) = c_T \eta^{-1/3} \left[ 3 \ln 3/2 + \pi \sqrt{3/6} + \ln(t/\eta) \right] t^{-2/3} \quad (t \gg \eta). \quad (13)$$

Hence the variance really decreases with time \cite{14}. The KP covariance must also be modified. Replacing $P(s)$ in Eq.(3) by $\mathcal{P}(s, t_0)$, where $t_0$ is an initial time, and evaluating integrals we get the effective covariance
where $W_{\alpha,\beta}(x)$ is the Whittaker function \[^{[15]}\] . This result is quite different from the original covariance \[^{[2]}\] and explains why the simulation does not agree with the analytical prediction \[^{[1]}\] . $C_{KP}(t, t_0) \sim t^{-1}$ for large $t$ but it depends also on $t_0$.

The above conclusions imply that problems involving algebraic correlations (e.g. critical phenomena, hydrodynamics), investigated in the framework of the Langevin description, should be handled with caution. Conversely, an experimental evidence of declining variance in such systems does not necessarily mean that Langevin formalism obeying standard fluctuation-dissipation theorems does not apply. In any individual case one should examine the distribution $P(s)$, the shape of which for large $s$ decides whether the system behaves in a stationary way. Is the stationary behaviour possible at all for correlations \[^{[2]}\] ? The analytical result would be valid for a steep $P(s)$. The fastest decaying distribution one can obtain with the KP for \[^{[2]}\] declines asymptotically like $s^{-2}$ \[^{[1]}\] . Since also for this distribution all moments diverge, we expect similar affects as for \[^{[1]}\] .

Another possibility is to apply a deterministic process, instead of the Markovian stochastic one. For that purpose, let us consider a two-dimensional lattice of periodically distributed disks of radius $r$, with a particle bouncing elastically from them. Then the particle motion is free between subsequent collisions and its velocity $\mathbf{u} = (u_x, u_y) = \text{const}$. This system, a periodic Lorentz gas, is equivalent to the Sinai billiard with periodic boundary conditions. We assume $2r < l$, where $l$ is the distance between disks centers. The system is strongly chaotic but the autocorrelation function of either component of particle velocity falls off slowly, as $1/t$ for large $t$ \[^{[1]}\] . Therefore we can simulate solutions of \[^{[1]}\] assuming the velocity of particle inside the independently evolved Sinai billiard as the stochastic force $F(t)$ \[^{[16]}\] . A quantity of interest is the distribution of free paths: it falls like $s^{-3}$ \[^{[17]}\] , steeper then for any KP. Its mean is convergent and the second moment weakly divergent. For numerical simulations we assume $l = 1$, $r = 0.8$, $|\mathbf{u}| = 1$ and $F = 7.3\sqrt{T}u_x$. Then $C_F = T/t$ for large $t$. We must stress, however, that the form of FAF at small $t$ also influences solutions of \[^{[1]}\] . Thus the simulations utilizing the Sinai billiard should be regarded as an approximation. The result of the numerical calculation of the variance $\langle v^2 \rangle(t)$ presents Fig.1. There are some discrepancies at small $t$, comparing to the analytical prediction, that can be attributed to differences in FAF. Asymptotically however, $\langle v^2 \rangle$ stabilizes at the equilibrium value and both results coincide, in contrast to the KP case.

Finally, we wish to calculate the velocity autocorrelation function (VAF) $C_v(t) = \langle v(t_0)v(t_0 + t) \rangle$, which is responsible for transport properties of the system. It allows us, namely, to determine the diffusion coefficient $D = \int_0^\infty C_v(t)dt$. Typically, $D$ is finite which corresponds to the normal diffusion. The analytical result for VAF in our case is \[^{[1]}\] : $C_v(t) = T/m \left[1 + \int_0^t R(\tau)d\tau\right]$. We present this function in Fig.2. It has the tail of the power-law shape with numerically estimated exponent equal to $-1.18$. On the other hand, we have calculated VAF from simulation utilizing the KP \[^{[18]}\] . The result for two values of $t_0$ is presented in Fig.2. We have normalized both functions to unity at $t = 0$. Their shape is very different from the analytical result. The VAF initially falls but then it stabilizes. It depends strongly on $t_0$, becoming more flat for larger $t_0$. The stationary case applying the Sinai billiard also produces result different from the analytical one $- C_v(t)$ is always non-negative and does not approach zero for increasing time. As regards the transport properties of the system, the analytical $C_v(t)$ implies the normal diffusion. Determination of
the precise shape of VAF at large $t$ for the KP and the simulation utilizing the deterministic random force, requires further studies. Anyway, it is obvious that the tails of VAF are very flat. Then the integration of VAF must produce a divergent result and $D$ becomes infinite, leading to the diffusion process anomalously enhanced. This result agrees with that obtained in the framework of the continuous-time random walk approach \cite{19} (Lévi walks) predicting the enhanced diffusion for power-law distributions of free paths; for (5) the motion becomes ballistic: $D$ diverges linearly with time.
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**Figure captions**

FIG. 1. The velocity variance calculated from Eq. [4] (solid line) and resulted from both simulations: with the KP (dashed line) and using the deterministic random force (dots). The parameters: \( T = 1 \), \( m = 1 \) and \( \epsilon = 0.01 \).

FIG. 2. The velocity autocorrelation function calculated using the KP with \( t_0 = 1.5 \) (dot-dashed line) and \( t_0 = 3 \) (dashed line), normalized to unity at \( t = 0 \). The result of the simulation with the deterministic random force is marked by dots. The solid line shows the analytical result. The parameters are the same as in Fig.1.
