Nonstationarity Induced by Long-Time Noise Correlations in the Langevin Equation

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We solve the generalized Langevin equation driven by a stochastic force with a power-law autocorrelation function. A stationary Markov process has been applied as a model of the noise. However, the resulting velocity variance does not stabilize but diminishes with time. It is shown that algebraic distributions can induce such effects. 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 the 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 a 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 [1,2] and the linearized hydrodynamics [3]. For such phenomena as the noise-induced Stark broadening [4] and nuclear collisions [5], 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 [6].

For systems with finite noise correlation time, the ordinary Langevin equation must be generalized to ensure proper fluctuation-dissipation relations [7]. The generalized Langevin equation has been introduced by Mori [8], later independently derived by Lee [9], as a useful description of many-body Hermitian systems. In the absence of external potential, this equation has the form

$$m\frac{dv(t)}{dt} = -m\int_0^t K(t-\tau)v(\tau)\,d\tau + F(t), \qquad (1)$$

where $F(t)$ is a stochastic force and $K(t)$ denotes the retarded friction kernel. The stochastic force describes deviations from an average motion due to nonlinear effects, the initial transient process, and fluctuations [8]. A direct solution of Eq. (1) is possible for some many-body systems, e.g., an electron gas model and a spin van der Waals model [10]. The fluctuation-dissipation theorem imposes the relation [11]: $K(t) = \langle F(0)F(t)\rangle_S/mT$, with temperature T and mass m. The average $\langle\,\rangle_S$ is taken over an equilibrium ensemble, with a stationary probability distribution. We assume that $F(t)$ can be an arbitrary random function satisfying the condition $\langle F(t)\rangle_S = 0$ and possessing the following covariance:

$$C_F(t) \equiv \langle F(0)F(t)\rangle_S = \begin{cases} \beta T/\epsilon & \text{for } t \le \epsilon \\ \beta T/t & \text{for } t > \epsilon \end{cases}, \qquad (2)$$

where ϵ is a small number. The coefficient β we set equal to one. The solution of Eq. (1) with the initial condition $v(0) = 0$ takes the form [12]

$$v(t) = g(t) + \int_0^t R(t-\tau)g(\tau)\,d\tau, \qquad (3)$$

where $g(t) = m^{-1}\int_0^t F(\tau)\,d\tau$ and the resolvent is given by $R(t) = \exp(-at)(c_1\sin bt + c_2\cos bt) + m\int_0^\infty x\exp(-tx)/\{[mx + \mathrm{Ei}_1(\epsilon x) - 1]^2 + \pi^2\}\,dx$. The modified integral exponential function $\mathrm{Ei}_1(x)$ is defined by the series: $\mathrm{Ei}_1(x) = \gamma + \ln x + \sum_{n=1}^\infty x^n/n!\,n$, where $\gamma = 0.577\,215\,7\ldots$ is the Euler constant. The other constants are fixed in the following at the values: $a = -3.528\,32$, $c_1 = -4.766\,73$, $c_2 = -5.354\,98$, and $b = 2.499\,75$, corresponding to $\epsilon = 0.01$ and $m = 1$.

The stochastic trajectories are not yet determined by Eq. (3) since the force $F(t)$ is not completely defined by its first two moments. However, some average quantities depend only on FAF and can be derived. In the following, we will refer to those results as "formal solutions" (FS). In particular, the FS for the second moment of the velocity distribution, $\langle v^2\rangle_S(t)$, can be obtained directly from (3):

$$\langle v^2\rangle_S(t) = 2\int_0^t d\tau\,(t-\tau)C_F(\tau) + 2\int_0^t d\tau\int_0^t ds_1\int_0^\tau ds_2\,R(t-\tau)C_F(|s_1-s_2|) + \int_0^t d\tau\int_0^t ds\int_0^\tau ds_1\int_0^s ds_2\,R(t-\tau)R(t-s)C_F(|s_1-s_2|). \qquad (4)$$

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.

Alternatively, we can introduce a concrete stochastic process possessing the properties required for $F(t)$, simulate stochastic trajectories by a Monte Carlo method, and calculate $\langle v^2\rangle_S$ averaging over those trajectories. We apply the "kangaroo process" (KP). It is defined [13] as a stepwise random function: $F(t) = F_i = \text{const}$ in the time interval $t_i \le t < t_{i+1}$. The length of interval of constant F, s, is a function of the value of the process

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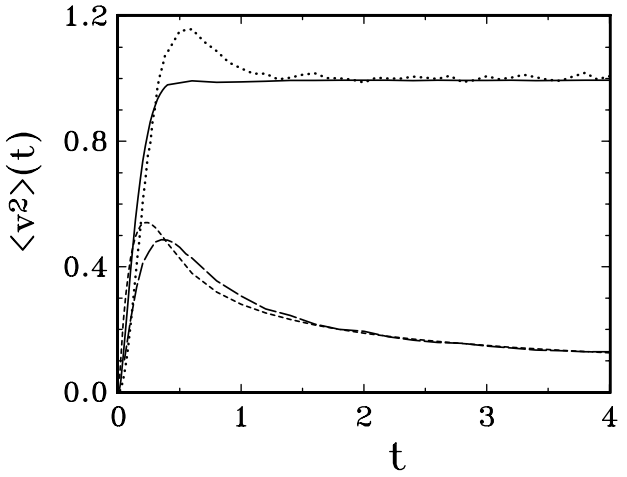

FIG. 1. The velocity variance calculated from Eq. (4) (solid line) and resulted from both simulations, with the KP (long-dashed line) and using the deterministic random force (dots). The short-dashed line shows $\langle v^2\rangle_S(t)$ calculated from Eq. (4) with the effective temperature $\hat{T}(t) = c_T\hat{\sigma}^2(t)$, where $c_T = 0.34$. The other parameters: $T = 1$, $m = 1$, and $\epsilon = 0.01$.

itself. The KP is a stationary Markov process, determined by a stationary probability distribution $P_{\mathrm{KP}}(F)$. It can be easily defined for arbitrary covariance. We get [14] the required form (2) by choosing $P_{\mathrm{KP}}(F) = 1/(2a) = \text{const}$ for $F \in (-a, a)$, zero elsewhere, where $a = \sqrt{3/\eta}$ with $\eta = \epsilon/T$. The time increment corresponding to a given F follows from the formula $s = 3a|F|^{-3}$. Thus s assumes values between η and infinity and its density distribution is of the form

$$P(s) = (\eta^{1/3}/3)s^{-4/3}\theta(s - \eta), \tag{5}$$

where $\theta(x)$ is the step function. Moments of F can easily be obtained by averaging over the uniform distribution $P_{\mathrm{KP}}(F)$. We get $\langle F\rangle_S = 0$ and $\sigma^2 \equiv \langle F^2\rangle_S = 1/\eta$. Since $2P_{\mathrm{KP}}(|F|)d|F| = P(s)ds$, we can average also over $P(s)$:

$$\sigma^2 = 3\eta^{-1/3}\int_0^\infty s^{-2/3}P(s)\,ds, \tag{6}$$

with the same result. Also the KP covariance [13,14], C_{KP}, can be expressed in terms of the distribution $P(s)$

$$C_{\mathrm{KP}}(t) = 3\eta^{-1/3}\int_0^\infty s^{-2/3}\exp(-t/s)P(s)\,ds. \tag{7}$$

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. Figure 1 presents the result: $\langle v^2\rangle_S$ does not stabilize at the expected value $\langle v^2\rangle_S = T/m$, but instead it dwindles with time, obeying the approximate relation $\langle v^2\rangle_S(t) \sim t^{-0.67}$.

The above outcome is surprising because, according to (4), $\langle v^2\rangle_S$ is completely determined by the covariance of F and every simulation satisfying (2) should reproduce the FS. In order to understand the origin of that inconsistency, let us reconsider in detail how the stochastic force value actually 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 $\hat{P}(s,t)$, 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 $s \le t$ and assume that t is found in $n+1$ interval, i.e., $S_n \equiv s_1 + s_2 + \cdots + s_n < t$ and $S_{n+1} > t$. The probability that the sum of n intervals yields a value between x and $x + dx$ we denote by $P_n(x)dx$, provided 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/η: $\Phi(s,t) = \sum_{n=1}^{N}\int_{t-s}^{t} P_n(x)\,dx\int_{t-x}^{s} P(\xi)\,d\xi$. Introducing $S(x) = \sum_{n=1}^{N} P_n(x)$ and inserting $P(x)$ from (5), we get the following equation:

$$\Phi(s,t) = \eta^{1/3}\int_{t-s}^{t} S(x)[(t-x)^{-1/3} - s^{-1/3}]\,dx \quad \text{for } \eta \le s \le t. \tag{8}$$

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:

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

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

$$\int_0^t S(x)\,(t-x)^{-1/3}\,dx + t^{-1/3} = \eta^{-1/3}, \tag{10}$$

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 [15]. The solution is of the form

$$S(x) = c_\Gamma\eta^{-1/3}x^{-2/3} - \delta(x), \tag{11}$$

where a constant $c_\Gamma = 1/[\Gamma(1/3)\Gamma(2/3)] \approx 0.2757\ldots$ 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 required probability distribution $\hat{P}(s,t)$, we have to differentiate $\Phi(s,t)$ over s. The final result is simple:

$$\widehat{P}(s,t) = \begin{cases} c_\Gamma[t^{1/3} - (t-s)^{1/3}]s^{-4/3} & \text{for } \eta \le s \le t \\ (c_\Gamma t^{1/3} + \eta^{1/3}/3)s^{-4/3} & \text{for } s > t \end{cases}. \tag{12}$$

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 meantime we must wait for a bus, providing we know the average time interval between subsequent bus arrivals (τ). The answer is not $\tau/2$, as one could expect, but just τ. This "waiting-time paradox" [16] 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 equilibrization, and the effective distribution asymptotically becomes time independent. For $\widehat{P}(s,t)$ it never happens. Moreover, since the probability $\widehat{P}(s > t, t) = \int_t^\infty \widehat{P}(s,t)\,ds = 3c_\Gamma \approx 0.83$ 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 $\widehat{P}(s,t)$, 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 $\hat{\sigma}^2(t)$, we can use Eq. (6) substituting $\widehat{P}(s,t)$ for $P(s)$. Evaluation of the integral gives us the final formula

$$\hat{\sigma}^2(t) = c_\Gamma \eta^{-1/3}[3\ln 3/2 + \pi\sqrt{3}/6 + \ln(t/\eta)]t^{-2/3} \quad (t \gg \eta). \tag{13}$$

Hence the variance really decreases with time [17]. The KP covariance must also be modified. Replacing $P(s)$ in Eq. (7) by $\widehat{P}(s,t_0)$, where t_0 is an initial time, and evaluating integrals we get the effective covariance

$$\widehat{C}_{\mathrm{KP}}(t,t_0) = c_\Gamma \eta^{-1/3} t_0^{1/3} t^{-1}[3 - \exp(-t/2t_0)\Gamma(1/3) \times W_{-1/3,-1/2}(t/t_0)], \tag{14}$$

where $W_{\alpha,\beta}(x)$ is the Whittaker function [18]. This result is quite different from the original covariance (2) and explains why the simulation does not agree with the FS (4). $\widehat{C}_{\mathrm{KP}}(t,t_0) \sim t^{-1}$ for large t, but it depends also on t_0. On the other hand, according to Eq. (4) the velocity variance is proportional to the temperature $T = \epsilon\sigma^2$. The declining of $\hat{\sigma}^2$ with time means that T can no longer be regarded as a constant parameter. Instead we can define an effective temperaturelike time-dependent function $\widehat{T}(t) = c_T\hat{\sigma}^2(t)$, where the constant c_T has been introduced to ensure a proper normalization, and modify the FS. The shape of the resulting function, presented in Fig. 1, is asymptotically the same as for the Monte Carlo simulation. Both curves coincide in this region for $c_T = 0.34$.

The above conclusions imply that the FS may not be a correct prediction for some problems involving algebraic correlations (e.g., critical phenomena, hydrodynamics). Accordingly, they should be handled with caution. Conversely, an experimental evidence of declining variance in such systems does not necessarily mean that the 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 velocity variance equilibrates at a finite value. Is such behavior possible at all for the covariance (2)? The FS 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} [14]. Since also for this distribution all moments diverge, we expect similar effects as for (5).

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 disk 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 [6]. Therefore we can simulate solutions of Eq. (1) assuming the velocity of particle inside the independently evolved Sinai billiard as the stochastic force $F(t)$ [19]. Its initial value has been chosen on a circle with a uniform, time-invariant, probability distribution. A quantity of interest is the distribution of free paths: it falls like s^{-3} [20], steeper than 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 $\langle v^2\rangle_S(t)$ presents Fig. 1. There are some discrepancies at small t, comparing to the FS, that can be attributed to differences in FAF. Asymptotically however, $\langle v^2\rangle_S$ stabilizes at the finite equilibrium value and both results coincide, in contrast to the KP case.

Finally, we wish to calculate the velocity autocorrelation function (VAF) $C_v(t) = \langle v(t_0)v(t_0 + t)\rangle_S$, which usually does not depend on t_0. This quantity is responsible for transport properties of the system. It allows us, namely, to determine the diffusion coefficient $\mathcal{D} = \int_0^\infty C_v(t)\,dt$. Typically, $\mathcal{D}$ is finite which corresponds to the normal diffusion [21]. The FS for VAF in our case is [12] $C_v(t) = T/m[1 + \int_0^t R(\tau)\,d\tau]$ and it does not depend on t_0. We present this function in Fig. 2. It has the tail of the

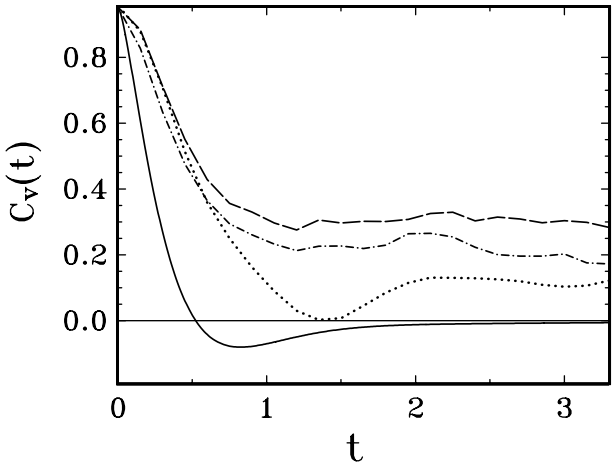

FIG. 2. The velocity autocorrelation function calculated using the KP with $t_0 = 1.5$ (dot-dashed line) and $t_0 = 3$ (dashed line), normalized to unity at $t = 0$. The result of the simulation with the deterministic random force is marked by dots. The solid line shows the FS. The parameters are the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

power-law shape with numerically estimated exponent equal to -1.18. On the other hand, we have calculated VAF from simulations utilizing the KP [22]. 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 FS. The VAF initially falls but then it stabilizes. Now it depends strongly on t_0, becoming more flat for larger t_0. The case applying the Sinai billiard, characterized by the finite, time-independent variance, also produces a result different from the FS $-$ $C_v(t)$, is always non-negative, and does not approach zero for increasing time. As regards the transport properties of the system, the FS 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 $\mathcal{D}$ becomes infinite, leading to the diffusion process anomalously enhanced. This result agrees with those obtained in the framework of a continuous-time random walk approach [23] (Lévi walks) and a stochastic collision model [24]. Both those approaches predict the enhanced diffusion for power-law distributions of free paths; for (5) the motion becomes ballistic: $\mathcal{D}$ diverges linearly with time.

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