Non-Markovian Brownian dynamics and nonergodicity

Jing-Dong Bao,[1] Peter Hänggi,[2] and Yi-Zhong Zhuo[3]
[1]*Department of Physics, Beijing Normal University, Beijing 100875, China*
[2]*Department of Physics, University of Augsburg, Universitätsstrasse 1, 86135 Augsburg, Germany*
[3]*China Institute of Atomic Energy, P.O. Box 275, Beijing 102413, China*

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We report the breaking of ergodicity for a class of generalized, Brownian motion obeying a non-Markovian dynamics being driven by a generalized Langevin equation (GLE). This very feature originates from a vanishing of the effective friction. A novel quantity b (being uniquely determined from the corresponding memory friction kernel $\gamma(t)$ of the GLE) is introduced as a parameter that is capable of measuring the strength of ergodicity breaking. The ergodicity breaking is accompanied by a nonunique stationary probability density for the corresponding embedded Markovian dynamics. Differing physical situations for a Brownian, non-Markovian particle dynamics occurring either in free Brownian motion, in a periodic potential, or in a confining potential are elucidated.

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I. INTRODUCTION

Ergodicity is a central concept in statistical physics: it states that the ensemble average of an observable quantity is equal to its time average in the infinite-time limit. This implies further a unique asymptotic, generally stationary state for the correspondingly embedded stochastic dynamics [1,2]. The ergodic hypothesis has been investigated experimentally in two different systems governed by Lévy statistics in time: fluorescence intermittency of nanocrystal quantum dots [3] and subrecoil laser cooling of atoms [4]. Very recently, Lutz [5,6] has established an explicit correspondence between ergodicity breaking and the divergence of the moments of the power-law tail distributions describing the behavior of the system. Until now most of the examples for ergodicity breaking are with the divergence of their first and second moments leading to nonstationarity [5,7], i.e., to a situation for which the breaking of ergodicity is expected.

The objective which we address in this paper is whether ergodicity can be broken in systems that are driven by non-Markovian Brownian motion processes. Many realistic physical stochastic processes fail to be ideally Markovian although they may be Gaussian. In recent years, there has been growing interest in anomalous diffusion in various fields of physics and related areas in science, where the ballistic diffusion is the limit of superdiffusion. It can be realized with a Gaussian non-Markovian process described by a generalized Langevin equation (GLE) [8–11]. The mean-square displacement of individual particles grows proportional to the square of time and these should exhibit a noise-driven *acceleration* when a constant force is applied. This constitutes an intermediate situation between the Newton mechanics (determinate) and a Langevin formalism (stochastic). Moreover, the validity of the fluctuation-dissipation theorem (FDT) is necessary, but not sufficient to yield a consistent thermal Brownian motion [12].

In this work, we are aiming at identifying a condition that necessarily leads to ergodicity breaking for a non-Markovian dynamics which is either free, or takes place in a periodic or confining potential landscape. A parameter measuring the nonergodicity strength is proposed for the analysis of generally preparation-dependent, asymptotic results. Furthermore, we specify various physical situations for which the stationary behavior is not unique.

II. GENERALIZED LANGEVIN EQUATION

The motion of a particle with mass μ subjected to a thermal colored noise [13] $\varepsilon(t)$ is described by a GLE,

$$\mu\dot{v}(t) + \mu\int_0^t \gamma(t-t')v(t')dt' + U'(x) = \varepsilon(t), \tag{1}$$

where $\gamma(t)$ is the memory friction kernel, $U(x)$ denotes the potential for the Brownian particle motion. The generally colored noise $\varepsilon(t)$ is of vanishing mean and is not correlated with the initial velocity. Its stationary correlation satisfies Kubo's second FDT, expressed as $\langle\varepsilon(t)\varepsilon(0)\rangle = \mu k_B T\gamma(t)$ [14,15]. Here, k_B is the Boltzmann constant and T is the temperature of the heat bath.

When the potential is absent, i.e., we deal with free Brownian motion [15], the solution of Eq. (1) can be obtained by means of the Laplace transform technique, i.e.,

$$v(t) = R(t)v_0 + \mu^{-1}\int_0^t R(t-t')\varepsilon(t')dt', \tag{2}$$

with v_0 being the initial velocity of the particle. The response function $R(t)$ follows from the inverse Laplace transform, denoted by $\hat{R}(z)=[z+\hat{\gamma}(z)]^{-1}$, where $\hat{\gamma}(z)$ is the Laplace transform of the memory friction kernel. Because the noise appearing in Eq. (1) is assumed to be Gaussian and the GLE is linear in the absence of a potential $U(x)$, the velocity probability density function (*pdf*) of the particle is also Gaussian; i.e.,

$$P(v,v_0,t) = \frac{1}{\sqrt{2\pi\sigma_v^2(t)}}\exp\left(-\frac{[v-R(t)v_0]^2}{2\sigma_v^2(t)}\right). \tag{3}$$

From Eq. (3) the time-convolutionless, generalized Fokker-Planck equation (FPE) for the velocity distribution can be derived in a straightforward manner [16]. The exact result for a free Brownian particle subjected to a Gaussian noise reads

$$\frac{\partial}{\partial t}P(v,v_0,t) = \tilde{\gamma}(t)\frac{\partial}{\partial v}[vP(v,v_0,t)] + \frac{k_B T}{\mu}\tilde{\gamma}(t)\frac{\partial^2}{\partial v^2}P(v,v_0,t) \tag{4}$$

with the time-dependent, effective friction $\tilde{\gamma}(t)=-\dot{R}(t)/R(t)$. We obtain the response function from the residue theory $R(t)=b+\Sigma_j\text{res}[\hat{R}(z_j)]\exp(z_j t)$, where

$$b = R(t\to\infty) = \{1 + \lim_{z\to 0}[\hat{\gamma}(z)/z]\}^{-1} \tag{5}$$

and z_j are nonzero roots of the equation $z+\hat{\gamma}(z)=0$. Note that the real parts of all roots are negative. This leads to $\tilde{\gamma}(t\to\infty)\to 0$ whenever $b\neq 0$, yielding the effective friction value $\hat{\gamma}(0)\equiv\int_0^\infty\gamma(t)dt=0$. This result also implies that the spectral power density of thermal noise $\varepsilon(t)$ is vanishing at zero frequency. Consequently, with such noise obeying $b\neq 0$, Eq. (4) does not reduce to the phenomenological FPE and, moreover, the system cannot approach asymptotically the equilibrium velocity solution with zero mean and the variance of k_BT/μ. Note, however, that a slow, longtime correlation does not necessarily imply a breaking of ergodicity: An important situation refers to non-Markovian Brownian motion within fluctuating hydrodynamics [17] with a non-Stokesian drag obeying a power-law response function, i.e., $R(t\to\infty)\sim t^{-3/2}$. This implies that $\lim_{t\to\infty}\tilde{\gamma}(t)=3/(2t)$. In this case, however, we find that $b=0$; therefore, the velocity equilibrium *pdf* is ensured [17].

III. ERGODICITY CRITERION FOR STOCHASTIC VARIABLES

A central problem in the theory of stochastic processes is the estimation of their statistics. Generally, we call a stochastic process $x(t)$ ergodic if its ensemble averages equal the corresponding time averages. This implies that any statistics of $x(t)$ can be inferred from a single realization. In most applications, however, we are interested in certain, specific statistics only, such as the mean, the second moment, or its correlation. A criterion for the ergodicity in the mean-square sense of a certain stochastic parameter, i.e., for the equality between ensemble average and time average of a stochastic observable $A(t)$, is provided by the following condition [5,6]: In particular, $A(t)$ is termed "mean"-ergodic, if $\lim_{t\to\infty}\sigma_A^2(t)=0$, with $\sigma_A^2(t)$ defined by

$$\sigma_A^2(t) = \frac{1}{t^2}\int_0^t dt_1\int_0^t dt_2[\{\langle A(t_1)A(t_2)\rangle\} - \{\langle A(t_1)\rangle\}\{\langle A(t_2)\rangle\}]. \tag{6}$$

Herein we indicate by $\{\ldots\}$ the average with respect to the initial values of the state variables and by $\langle\ldots\rangle$ we denote the average over the noise $\varepsilon(t)$, respectively.

As is well known, a Gaussian distribution is completely determined by its first two moments. For the present Gaussian non-Markovian process in Eq. (3), we take $A(t)=v(t)$ and $v^2(t)$. If $b\neq 0$ and $\neq 1$ the longtime behavior of the two corresponding "ergodicity" quantifiers emerge as

$$\sigma_v^2(t\to\infty) = \mu^{-1}k_BTb(1-b)\neq 0 \tag{7}$$

and

$$\sigma_{v^2}^2(t\to\infty) = 2\mu^{-1}k_BTb^2(1-b)[\mu^{-1}k_BT(1-b)+2\{v_0^2\}b]\neq 0. \tag{8}$$

We can assess that ergodicity is assumed for Gaussian anomalous diffusion obeying $b=0$ and deterministic Newton mechanics with $b=1$.

Alternatively, according to the Khinchin's theorem, a unified criterion for ergodicity is related to the asymptotical behavior of velocity correlation function [2,6]. Within our modeling of free Brownian motion, the velocity correlation function in the asymptotic longtime limit emerges as

$$\lim_{t\to\infty}\{\langle v(t)v(0)\rangle\} = \{v_0^2\}b^2 + k_BT\mu^{-1}b(1-b)\neq 0. \tag{9}$$

This implies that the condition for ergodicity from Khinchin's theorem [2,6] does not hold when $b\neq 0$. It is for this fact that the measure b (for "breaking") is adopted as the parameter measuring the nonergodicity strength b.

IV. STOCHASTIC SYSTEMS WITH NONERGODIC BEVAVIOR

In the following we elucidate a few physical situations where ergodicity can be broken and evaluate the corresponding nonergodicity strength b.

(i) We start out by considering a simple coupled classical Hamiltonian system, i.e., a free particle that is coupled bilinearly to the velocity variable of a harmonic oscillator; see also in Refs. [18] and [19] for more general velocity-type couplings. The Hamiltonian then reads

$$H = \frac{1}{2}\mu\dot{x}^2 + \frac{1}{2}\alpha[\dot{q}^2+\omega^2q^2] + cx\dot{q}, \tag{10}$$

where c is the coupling constant. The equation of motion of the $x(t)$ process is given by

$$\mu\ddot{x}(t) + \frac{c^2}{\alpha}\int_0^t \cos\omega(t-s)\dot{x}(s)ds = \xi(t), \tag{11}$$

where $\xi(t)=c[-\omega q(0)\sin\omega t+\dot{q}(0)\cos\omega t]$. If both $q(0)$ and $\dot{q}(0)$ are assumed to be two independent random variables which obey a Gaussian distribution with $\langle q(0)\rangle=\langle\dot{q}(0)\rangle=0$, $\omega^2\langle q^2(0)\rangle=\langle\dot{q}^2(0)\rangle=D/\alpha$, and $\langle q(0)\dot{q}(0)\rangle=0$. Thus, $\langle\xi(t)\xi(s)\rangle=Dc^2\alpha^{-1}\cos\omega(t-s)$. We yield the nonergodic parameter b, reading $b=[1+c^2(\omega^2\alpha\mu)^{-1}]^{-1}$. Therefore, the reduced dynamics $x(t)$ is nonergodic.

(ii) As another case, let us consider a one-electron atom with mass μ and charge e interacting with the radiation field in the dipole approximation [20,21], corresponding to the following Hamiltonian:

$$H = \frac{1}{2m}\left[\mathbf{p} + \frac{e}{c}\mathbf{A}\right]^2 + U(\mathbf{r}) + \sum_{\mathbf{k},s} \hbar\omega_{\mathbf{k}}\left(a^+_{\mathbf{k},s}a_{\mathbf{k},s} + \frac{1}{2}\right) \tag{12}$$

with the vector potential given by

$$\mathbf{A} = \sum_{\mathbf{k},s}\left(\frac{2\pi\hbar c^2}{\omega_{\mathbf{k}}V}\right)^{1/2} f_{\mathbf{k}}\hat{\mathbf{e}}_{\mathbf{k},s}(a_{\mathbf{k},s} + a^+_{\mathbf{k},s}), \tag{13}$$

where the quantity $f_{\mathbf{k}}$ is the electron form factor, $\hat{\mathbf{e}}$ enotes the polarization, and V is the volume [20,21]. The electrodynamic Hamiltonian (12) is a three-dimensional version of the velocity coupling Hamiltonian. The parameter b is then evaluated as

$$b = [1 + 2e^2\Omega/(3c^3\mu)]^{-1}, \tag{14}$$

where Ω is a large cutoff frequency. If the particle carries no charge, i.e., $e=0$, we have $b=1$, meaning that the damping of the particle for this the black-body radiation field is induced by its charge.

(iii) Next, we consider an acoustic phonon model proposed in Refs. [9] and [10], where a criterion has been presented in order to produce ballistic diffusion when the low-frequency part of the density of states of the thermal bath is removed. The spectral density of noise is then given by $\rho_n(\omega)=C$, for $\omega_1 < \omega < \omega_s$; and 0 otherwise, where C is a constant. This noise originates from a coupled harmonic chain, where ω_s is the Debye phonon frequency and ω_1 is a typical frequency. Here

$$b = [1 + C(\omega_1^{-1} - \omega_s^{-1})]^{-1}. \tag{15}$$

(iv) Yet another situation occurs for an inertia ratchet with coexisting regular attractors [22]; then, the diffusion behavior of a Brownian motor emerges also as being ballistic with a second moment that grows proportional to the square of time. These inertial ratchet trajectories thus seem to mimic the behavior of the free, nonergodic Brownian motion behavior in the absence of a potential. The nonergodicity strength can be determined by the curvature of the mean-square displacement of the particle.

In practice, in all those situations discussed above, the spectral power density of corresponding thermal colored noise is causing an ergodicity breaking; it is rooted in the vanishing weight at zero frequency. Moreover, any realistic spectral density of noise decays in the limit $\omega \to \infty$, because physical quantities seemingly should not diverge. Both of these conditions imply that the noise is colored with a limiting *band-passing* behavior at large frequencies.

V. MODELING ERGODICITY BREAKING COLORED NOISE

We next propose an archetype band-passing colored noise which can be realized from an m-order derivative $y^{(m)}(t)$ of the solution of a linear n-order stochastic differential equation driven by a Gaussian white noise $\xi(t)$ of strength $D=2k_BT\gamma\mu$; i.e.,

$$a_n\frac{d^n}{dt^n}y(t) + a_{n-1}\frac{d^{n-1}}{dt^{n-1}}y(t) + \cdots + a_0 y(t) = \xi(t), \tag{16}$$

with $m \leq n$. The colored noise is termed "green" when $m=n$, since the spectrum of noise approaches a constant in the limit of high frequency.

Typically, the process obtained from the solution of this linear stochastic differential equation driven by a Gaussian white noise is regarded as a noise source [23]. For example, the case $y^{(m=0)}(t)$ with $n=1$ corresponds to Ornstein-Uhlenbeck noise and the case with $n=2$ to harmonic noise, respectively [24]. Here, the m-order derivative $y^{(m)}(t)(1 \leq m \leq n)$ of the solution is used as the source of colored thermal noise that drives the GLE, i.e., $\varepsilon(t)=y^{(m)}(t)$ in Eq. (1), with $\gamma_m(t-t')$ denoting the corresponding memory kernel function through the Kubo second FDT [14], i.e.,

$$\gamma_m(t-s) = \frac{1}{\mu k_B T}\langle y^{(m)}(t)y^{(m)}(s)\rangle,$$
$$= \int_{-\infty}^{\infty} d\omega \frac{\alpha\omega^{2m}}{|\chi_n(\omega)|^2}\exp[i\omega(t-s)], \tag{17}$$

where the coefficient α is determined as $\alpha=\gamma a_m^2$ [19] and γ is the friction parameter corresponding to the thermal white noise, cf. above Eq. (16). $\chi_n(\omega)$ is a polynomial in ω, given by

$$\chi_n(\omega) = a_n(i\omega)^n + a_{n-1}(i\omega)^{n-1} + \cdots + a_0. \tag{18}$$

Upon observing (16), we next introduce in (1) the variable $w_1=-\int_0^t dt'\gamma_m(t-t')v(t')$ together with the auxiliary variables: $w_2,\ldots,w_n$ in the following. In doing so, we obtain a $2(n+1)$-dimensional Markovian embedding of the colored noise dynamics, reading

$$\dot{x} = v,$$
$$\mu\dot{v} = -a_n^{-2}\delta_{nm}v + w_1 - U'(x) + y^{(m)}(t),$$
$$\dot{w}_1 = -\gamma_m(0)v + w_2,$$
$$\cdots$$
$$\dot{w}_{n-1} = -\gamma_m^{(n-2)}(0)v + w_n,$$
$$\dot{w}_n = -\gamma_m^{(n-1)}(0)v - \frac{a_0}{a_n}w_1 - \cdots - \frac{a_{n-1}}{a_n}w_n, \tag{19}$$

where the values $\gamma_m^{(j)}(0)$ $(j=0,1,2,\ldots,n-1)$ denote the derivatives of order j at time 0 as obtained from Eq. (17).

The nonergodicity strength b is now evaluated to read

$$b = \frac{1}{1 + \frac{2}{\pi}\int_0^{\infty} d\omega \frac{\alpha\omega^{2m-2}}{|\chi_n(\omega)|^2}}. \tag{20}$$

For example, for the case with $n=1$, $b=(1+\gamma a_1/a_0)^{-1}$ if $m=1$, while $b=0$ for $m=0$. Likewise, for $n=2$,

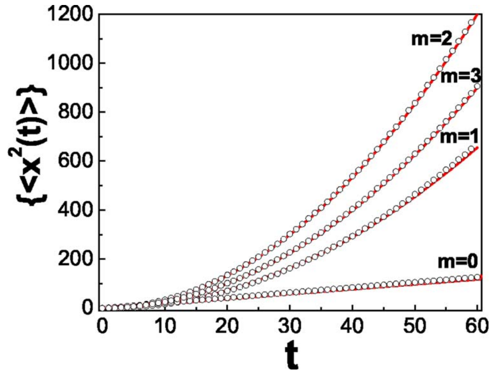

FIG. 1. (Color online) Time-dependent mean square displacement of a free particle for various values m at fixed $n=3$, see Eq. (16) and text. The open circles are numerical data and the solid lines depict the theoretical results [Eq. (20)]. The chosen parameters are $a_3=a_2=a_0=1$, $a_1=1.5$, $\gamma=1$, and $T=T_0=1$.

$b=(1+\gamma a_2^4/a_1)^{-1}$ if $m=2$, $b=(1+\gamma a_1/a_0)^{-1}$ if $m=1$, and ergodicity holds with $b=0$ for $m=0$.

A. Free, nonergodic Brownian motion

In Fig. 1, we depict for the embedded set of Markovian Langevin equations in (19) with $n=3$ the numerically evaluated diffusive behavior for the mean-square displacement $\langle x^2(t)\rangle$ for free (i.e., in the absence of a potential force) colored Brownian motion that starts out at $x(0)=0$ and $v(0)$ obeying a Gaussian distribution with zero mean and variance $\{v^2(0)\}=k_BT_0/\mu$, where T_0 is the initial temperature of system.

All quantities depicted therein, and in the forthcoming, are dimensionless (i.e., $k_B=1$ and $\mu=1$). As expected, we obtain normal diffusion for $m=0$; the diffusion, however, becomes ballistic for $1\leq m\leq 3$. Analytically we find for the asymptotic longtime behavior the result $\{\langle x^2(t)\rangle\}=[k_BT/\mu+b(\{v_0^2\}-k_BT/\mu)]bt^2$. Ballistic diffusion due to a vanishing effective friction mimics the limit of Brownian diffusion, and is intermediate between that induced by an internal Gaussian white noise in the presence of friction and an external white noise without friction. The asymptotic mean-square displacement of a free particle dynamics is proportional to t for normal diffusion and is proportional to t^3 for a frictionless, white-noise-driven dynamics. The t^3 diffusive behavior has been observed in two-dimensional turbulence, which is also called Richardson's law [25].

B. Brownian motion in a periodic potential driven by nonergodic noise

As another physical application, we consider generalized Brownian motion in a periodic potential. The particle subjected to a thermal green noise (i.e., $n=1$ and $m=1$) [26] and moving in a periodic potential: $U(x)=-U_0\cos(x)$. The time-dependent mean energy of the particle is given by

$$\{\langle E(t)\rangle\}=\frac{1}{2}m\{\langle v^2(t)\rangle\}+\{\langle U(x)\rangle\}. \tag{21}$$

This quantity is calculated numerically by using a Langevin Monte-Carlo simulation. The particle starts out from $x(0)=0$ and its initial velocity distribution is assumed to be a Gaussian with zero mean and variance k_BT_0/μ. The results are depicted in Fig. 2. Upon inspection, we find a prominent result: There exists a threshold for the potential barrier $U_{0,th}$ *below* which the ergodicity is broken. This threshold depends explicitly on the parameters of the colored noise. Namely, the stationary mean energy of the particle depends on its initial velocity variance. This threshold originates from the fact that with decreasing potential barrier the Brownian particles can increasingly surmount the potential and experience approximatively free diffusion without thermalization with the colored heat bath for U_0 less than $U_{0,th}$. On the other hand, with a large U_0 (above $U_{0,th}$) particles are predominantly localized in the low-energy region, where they experience the confining part of the potential. In this case, the mean energy of the particle is equal to a preparation-independent constant, thereby recovering ergodicity.

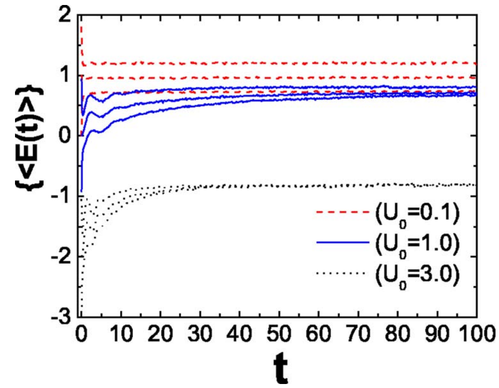

FIG. 2. (Color online) The mean energy of a particle in a periodic potential driven by a thermal green noise. The parameters used are $a_0=4$, $a_1=1$, $\gamma=4$, and $T=2$. At each group of lines, the initial temperatures of the particle are chosen to be $T_0=2T$, T, and 0 from top to bottom.

C. Brownian motion in a confining potential

For a harmonic potential $U(x)=\frac{1}{2}m\omega_0^2x^2$, where zero root does not exist for Laplace transforms of the response functions of both position degree of freedom $[(z^2+z\hat{\gamma}(z)+\omega_0^2)^{-1}]$ and velocity degree of freedom $[z\{z^2+z\hat{\gamma}(z)+\omega_0^2\}^{-1}]$. Thus, the coefficients appearing in generalized FPE [16] approach asymptotically constants. This leads to the result that the average energy of the particle at the stationary state is $\langle E\rangle_{\rm st}=k_BT$, independent of the initial distribution of the particle; i.e., ergodicity is obeyed.

VI. CONCLUSIONS

As demonstrated herein, we find that a breaking of ergodicity may occur for a Gaussian non-Markovian dynamics if the effective friction of the system vanishes at zero frequency or likewise, when the spectral density of thermal colored noise possesses a vanishing weight at zero frequency. For such nonergodic and non-Markovian processes, a characteristic feature emerges: the mean value, variance, and correlation function for velocity degree of freedom asymptotically become preparation dependent. This in turn implies a breakdown of ergodicity accompanied by a nonunique stationary state for the embedded process. The equilibrium state with a Gaussian of weight $k_B T$ needs to be connected with the Kubo second fluctuation-dissipation relation in order to yield ergodicity. We consider also the case of generalized Brownian motion in a periodic potential. Then, ergodicity is broken when the temperature strength is sufficiently larger than a threshold value that critically depends on the parameters of the ergodicity breaking colored noise; below threshold, the diffusion is normal and ergodicity is recovered.

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