# Nonergodic solutions of the generalized Langevin equation

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It is known that in the regime of superlinear diffusion, characterized by zero integral friction (vanishing integral of the memory function), the generalized Langevin equation may have nonergodic solutions that do not relax to equilibrium values. It is shown that the equation may have nonergodic (nonstationary) solutions even if the integral of the memory function is finite and diffusion is normal.

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There is hardly anything more important to say about a statistical mechanical system than whether it is ergodic or not. In general the question is notoriously difficult, yet for certain classes of stochastic systems the criteria of ergodicity breaking may be remarkably simple [1–5]. This is so, or so it would appear, for stochastic dynamics described by the generalized Langevin equation (GLE)

$$\frac{dA(t)}{dt} = -\int_0^t d\tau\, M(t-\tau)\,A(\tau) + F(t), \tag{1}$$

which governs a dynamical variable $A$ of a classical system coupled to a thermal bath with many degrees of freedom in the absence of external forces [6]. The "random" force $F(t)$ is zero centered $\langle F(t)\rangle = 0$, not correlated with the initial value of $A$:

$$\langle A(0)F(t)\rangle = 0, \tag{2}$$

and related with the dissipative memory function $M(t)$ through the fluctuation-dissipation theorem

$$\langle F(0)F(t)\rangle = \langle A^2\rangle\, M(t). \tag{3}$$

We shall also assume the asymptotic vanishing of correlations of the random force

$$\lim_{t\to\infty}\langle F(0)F(t)\rangle = \lim_{t\to\infty} M(t) = 0, \tag{4}$$

which is typical for irreversible stochastic processes. It appears to be a common belief that, given conditions (3) and (4), solutions of the GLE (1) describe ergodic relaxation to thermal equilibrium, unless the Laplace transform of the memory function $\tilde{M}(s) = \int_0^\infty dt\, e^{-st} M(t)$ has a specific asymptotic behavior. Namely, it was shown in Refs. [3–5] that the condition of ergodicity breaking for GLE systems has the form

$$\tilde{M}(s) \sim s^\delta, \quad \delta \geqslant 1, \quad \text{as } s \to 0. \tag{5}$$

This condition implies the vanishing integral of the memory function

$$\int_0^\infty dt\, M(t) = \tilde{M}(0) = 0. \tag{6}$$

If the targeted variable $A$ is the velocity of a Brownian particle, condition (6) corresponds to anomalous diffusion when the mean-square displacement $\langle x^2(t)\rangle$ of the particle increases with time as $t^\alpha$ with $\alpha > 1$ (superdiffusion) [8,9]. The relation (6) is not very common, but not unrealistic. For instance, it was found to hold for a particle interacting with longitudinal phonons in liquids in the limit of zero temperature [10]. It should perhaps be noted that while the condition of ergodicity breaking (5) invariably implies superdiffusion, the converse is not true: For $\tilde{M}(s) \sim s^\delta$ with $0 < \delta < 1$ the condition of superdiffusion (6) is satisfied, yet solutions of the GLE (1) are ergodic [3]; see also Eq. (12) below.

The purpose of this paper is to show that the condition of ergodicity breaking in the form (5) is too restrictive. It will be demonstrated that the GLE may have nonergodic solutions even if the memory function does not follow the asymptotic form (5), $\tilde{M}(0) = \int_0^\infty M(t)\, dt$ is finite, and diffusion is normal.

We begin by briefly recapitulating the derivation of condition (5), which may differ depending on a type of averaging $\langle \ldots \rangle$ in relations (2) and (3). When the GLE is derived with the Mori's projection operator technique [6], the system is usually assumed to be in thermal equilibrium with the bath, and the averaging in Eqs. (2) and (3) is over the ensemble of initial conditions for the composition of the system and the bath in mutual thermal equilibrium. In this case it is natural to use the GLE to evaluate the equilibrium correlation function $\langle A(0)A(t)\rangle$. Its normalized form

$$C(t) = \frac{\langle A(0)A(t)\rangle}{\langle A^2(0)\rangle} \tag{7}$$

satisfies the equation

$$\frac{dC(t)}{dt} = -\int_0^t d\tau\, M(t-\tau)\, C(\tau) \tag{8}$$

with the initial condition $C(0) = 1$ and has a Laplace transform

$$\tilde{C}(s) = \frac{1}{s + \tilde{M}(s)}. \tag{9}$$

The connection to ergodic properties is given by Khinchin's theorem [7] (see also Ref. [2]), which states that the stationary process $A(t)$ is ergodic if the correlation function factorizes and, for a zero-centered process, vanishes in the long-time limit

$$\lim_{t\to\infty} C(t) = \frac{\langle A(0)\rangle\langle A(t)\rangle}{\langle A^2(0)\rangle} = 0. \tag{10}$$

Although in Mori's GLE the random force $F(t)$, and therefore $A(t)$, are not necessarily stationary and zero centered, we shall

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assume that these properties do hold. Then Eqs. (9), (10), and the limit value theorem

$$\lim_{t\to\infty} C(t) = \lim_{s\to 0} s\,\tilde{C}(s) \quad (11)$$

give the condition of ergodicity breaking in the following form:

$$\lim_{s\to 0} \frac{s}{s+\tilde{M}(s)} \neq 0, \quad (12)$$

which leads to condition (5).

A slightly different approach is to apply for a particular and very popular class of models where the random force $F(t)$ does not depend on $A$. This is the case, for instance, when $A$ is the momentum of a Brownian particle that is bilinearly coupled to the bath comprising harmonic oscillators [6]. For this problem, often referred to as the Caldeira-Leggett model, relation (2) is satisfied trivially, the random force is stationary (for the infinite bath), and the fluctuation dissipation theorem takes the form

$$\langle F(0)F(t)\rangle_0 = \langle A^2\rangle\, M(t), \quad (13)$$

where the the average $\langle\ldots\rangle_0$ is taken over bath variables only. The latter allows one to use the GLE to evaluate not only the equilibrium correlation function but also the second moment $\langle A^2(t)\rangle_0$, which characterizes the process of thermalization of the system, which at the moment $t=0$ is put in contact with the equilibrium thermal bath. Compared to Mori's approach, this is a more general problem since the initial equilibrium of the system and the bath is not assumed. One can show that the system does not thermalize,

$$\lim_{t\to\infty} \langle A^2(t)\rangle_0 \neq \langle A^2\rangle, \quad (14)$$

under the same condition as that for ergodicity breaking discussed above. Indeed, using a Laplace transformation the solution of the GLE (1) can be written in the form

$$A(t) = A(0)\,C(t) + \int_0^t d\tau\, C(t-\tau)\,F(\tau), \quad (15)$$

where the response function $C(t)$ has the transform given by Eq. (9) and therefore coincides with the correlation function for Mori's GLE and satisfies Eq. (8). By squaring and averaging solution (15) over bath variables, and also using stationarity of $F(t)$ and the fluctuation-dissipation relation (13)

$$\langle F(t_1)F(t_2)\rangle_0 = \langle A^2\rangle\, M(|t_1-t_2|), \quad (16)$$

one gets

$$\langle A^2(t)\rangle_0 = A^2(0)\,C^2(t) + 2\langle A^2\rangle \int_0^t d\tau_1 C(\tau_1)\int_0^{\tau_1} d\tau_2\, C(\tau_2)M(\tau_1-\tau_2). \quad (17)$$

Using (8), this equation can be written as

$$\langle A^2(t)\rangle_0 = A^2(0)\,C^2(t) - 2\,\langle A^2\rangle \int_0^t d\tau_1 C(\tau_1)\,\dot{C}(\tau_1),$$

and eventually one obtains [11]

$$\langle A^2(t)\rangle_0 = A^2(0)\,C^2(t) + \langle A^2\rangle\,[1-C^2(t)]. \quad (18)$$

The system does not thermalize if the response function does not vanish in the long time limit, $\lim_{t\to\infty} C(t)\neq 0$, which again gives the conditions (12) and (5).

The above reasoning was based on the limit value theorem (11) which is only valid if the system reaches a stationary state and the long time limit for $C(t)$ does exist. One might suggest that this is always the case provided the random force is irreversible in the sense that the correlation function $\langle F(0)F(t)\rangle$ and the memory kernel $M(t)$ vanish as $t\to\infty$. Let us show that this assumption is incorrect: It is possible to construct memory functions $M(t)$ that vanish at long times, but the corresponding functions $C(t)$, related to $M(t)$ by Eq. (8) or (9), do not have a long time limit. The condition of superdiffusion $\int_0^\infty M(t)\,dt = 0$ is not required.

As an example, let us consider a class of memory functions with the Laplace transform

$$\tilde{M}(s) = -s + \frac{s^2+\omega^2}{f(s)}, \quad (19)$$

where $\omega$ is real and $f(s)$ is an analytic function at $s=\pm i\omega$. The corresponding transform for the correlation or response function $C(t)$, given by (9), is

$$\tilde{C}(s) = \frac{f(s)}{s^2+\omega^2}. \quad (20)$$

It has simple poles at $s=\pm i\omega$ on the imaginary axis, and therefore the original $C(t)$ contains terms oscillating with frequency $\omega$ and does not reach a stationary value as $t\to\infty$. It is not immediately obvious, however, whether it is possible to construct a function $f(s)$ that ensures that the memory kernel behaves in a physically reasonable way. There are several conditions to satisfy. First, as a Laplace transform must vanish in the limit $s\to\infty$, we must require, in view of (19), that

$$f(s)\sim s, \quad \text{as } s\to\infty. \quad (21)$$

The second condition is the asymptotic vanishing of correlations (4),

$$\lim_{t\to\infty} M(t) = \lim_{s\to 0} s\,\tilde{M}(s) = 0, \quad (22)$$

which leads to the asymptotic constraint

$$f(s)\sim s^r, \quad r<1 \quad \text{as } s\to 0. \quad (23)$$

The third condition, which is more difficult to handle than the other two, is that the memory function must not exceed its initial value,

$$|M(t)| \leqslant M(0), \quad \text{for } t>0. \quad (24)$$

This is because $M(t)$ is essentially the correlation function of the stationary stochastic process $F(t)$, which satisfies the inequality

$$\langle [F(0)-F(t)]^2\rangle = 2\langle F^2(0)\rangle - 2\langle F(0)F(t)\rangle \geqslant 0.$$

Condition (24) cannot be formulated as that for the Laplace transform $\tilde{M}(s)$, which makes the choice of $f(s)$ in Eq. (19) not quite straightforward. It turns out that the simplest function $f(s)$ that can be made consistent with all three conditions (21), (23), and (24) is

$$f(s) = \frac{s^2+as+b}{s+c}, \quad (25)$$

with certain restrictions on the real constants $a$,$b$, and $c$. In this case

$$\tilde{C}(s) = \frac{s^2 + as + b}{(s + c)(s^2 + \omega^2)}, \tag{26}$$

while the transform of the the memory function (19) can be written in the form

$$\tilde{M}(s) = \alpha + \frac{\beta s + \gamma}{s^2 + as + b}, \tag{27}$$

where

$$\begin{aligned} \alpha &= c - a, \\ \beta &= \omega^2 - b - a(c - a), \\ \gamma &= \omega^2 c - b(c - a). \end{aligned} \tag{28}$$

The inverse Laplace transformation $\mathcal{L}^{-1}$ of (27) gives the memory function as a sum of the Dirac delta function and a nonsingular part,

$$M(t) = \alpha\, \delta(t) + m(t). \tag{29}$$

Conditions (22) and (24) are satisfied if the singular part is positive ($\alpha > 0$), and the nonsingular function

$$m(t) = \mathcal{L}^{-1}\left\{\frac{\beta s + \gamma}{s^2 + as + b}\right\} \tag{30}$$

vanishes as $t \to \infty$. This sets the constraints

$$c > a > 0, \quad b \neq 0, \tag{31}$$

while $\omega$ is still an arbitrary parameter.

As an illustration consider the set of parameters $a = b = 1$, $c = 2$, and $\omega^2 = 2$. Then Eqs. (28) give $\alpha = 1$, $\beta = 0$, $\gamma = 3$, and transforms (26) and (27) read

$$\begin{aligned} \tilde{M}(s) &= 1 + \frac{3}{s^2 + s + 1}, \\ \tilde{C}(s) &= \frac{s^2 + s + 1}{(s^2 + 2)(s + 2)}. \end{aligned} \tag{32}$$

Respectively, in this case the memory function is

$$M(t) = \delta(t) + 2\sqrt{3}\, e^{-t/2} \sin\left(\frac{\sqrt{3}}{2} t\right) \tag{33}$$

and satisfies both conditions (22) and (24), while the correlation or response function

$$C(t) = \frac{1}{2} e^{-2t} + \frac{1}{2} \cos(\sqrt{2}\, t) \tag{34}$$

does not reach a long time limit. Observe that the nonsingular part of the memory function $m(t)$ increases at $t = 0$. As one can check, for the given class of memory functions (19), and under restriction (4), the property $m'(0) > 0$ is generic. Therefore the presence of a singular term in $M(t)$ is essential: If the delta function is absent in (29) ($\alpha = 0$), then the condition (24) cannot be met.

Needless to say, the condition of superdiffusion $\int_0^\infty dt\, M(t) = \tilde{M}(0) = 0$ is not implied in our construction. It follows from (27) that $\tilde{M}(0) = \omega^2 c/b$, and so, unless $\omega = 0$, $\tilde{M}(0)$ is finite and diffusion is normal. Since $b \neq 0$ due to (31), the regime of subdiffusion $\lim_{s\to 0} \tilde{M}(s) = \infty$ [8] does not occur for memory functions of type (27).

Summarizing, it is shown that stochastic dynamics governed by the generalized Langevin equation may be nondissipative in the regime of normal diffusion, and thus superdiffusion is not a necessary condition for ergodicity breaking, as often assumed in literature. In our showcase example the memory function consists of a delta peak and a long, generally nonmonotonic tail. A possibility of nonergodic dynamics generated by a noise with physically more realistic nonsingular correlations remains to be examined. In this case the time-reversal symmetry requires that the exact memory and autocorrelation functions must be even in time [12]. Neither this additional constraint nor the condition of subdiffusion [divergence of $\tilde{M}(s)$ as $s \to 0$] can be met by the simple class of memory functions considered in this paper.

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