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Simple Measure of Memory for Dynamical Processes Described by a Generalized Langevin Equation

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Memory effects are a key feature in the description of the dynamical systems governed by the generalized Langevin equation, which presents an exact reformulation of the equation of motion. A simple measure for the estimation of memory effects is introduced within the framework of this description. Numerical calculations of the suggested measure and the analysis of memory effects are also applied for various model physical systems as well as for the phenomena of ''long time tails'' and anomalous diffusion.

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An abundant number of different problems involving molecular motion in condensed matter can be formulated in terms of the generalized Langevin equation (GLE). The latter can be exactly received in the context of the Zwanzig-Mori projection operator technique [1], as well as within the framework of the recurrent relation approach [2] from the equation of motion. As is known, this approach is used in the description of dynamical phenomena, ordinary and anomalous (such as anomalous diffusion) transport in physical, chemical, and even biophysical complex systems [1,3].

One of the key features of the GLE is the fact that it contains an aftereffect function, termed a memory function. If the memory function is delta function correlated (''a white noise''), the GLE is reduced to the ordinary Langevin equation corresponding to the system without memory, and the time correlation function (TCF) related to the momentum degree of freedom has simple exponential relaxation. So, a formalism based on GLE (and/or likewise, on the corresponding generalized Fokker-Planck equation) inherently contains *memory effects*, which characterize the system of interest [4].

Memory effects can appear in the velocity autocorrelation function (VACF) either through the presence of an oscillatory behavior or by means of slowly decreasing correlations. Thus, the memory character of the dynamics of liquids related to influence of the cage formed by nearest surroundings on the particle movement (the so-called ''cage effects'') belongs to the first case, whereas dynamical processes related to anomalous diffusion and long time tails in the behavior of TCF's correspond to the second situation. It is necessary to note that in the similar treatment the notion of ''memory'' is not completely definite. In particular, it is found that nonexponential relaxation [5] can be observed in glasses, simple fluids, and supercooled liquids [6], liquid crystals [7], plasmas [8], frustrated lattice gases [9], proteins [10], disordered vortex lattice in superconductors [11]. However, in concordance with GLE treatment, the process with memory effects constitutes *any* dynamical process, whose TCF decays at long times, according to a nonexponential law. As a result, the following questions arise. To what degree is the studied process not Markovian? Correspondingly, how large is the difference between the relaxation with memory and an exponential relaxation? How strong are the space and time nonlocality effects in the system? The situation would become more clear via the characterization by an adequate quantity [12], which would provide a numerical measure of manifest memory effects. In this Letter we present such a measure: it is obtained by comparing the time scales of the decay of the VACF and its corresponding memory function.

Thus, the GLE of Mori-type can be written as [2,3]:

$$m\frac{d}{dt}v_\alpha(t) = -m\omega^{(2)}\int_0^t M_1(t-\tau)v_\alpha(\tau)d\tau + F(t), \quad (1)$$

where $\omega^{(2)} = \langle|\mathcal{L}v_\alpha|^2\rangle/\langle|v_\alpha|^2\rangle$ is the second frequency moment of VACF with the Liouville operator $\mathcal{L}$, and the normalized memory function $M_1(t)$ can be related to the stochastic force $F(t)$ by means of the fluctuation-dissipation theorem, $\langle F(t)F(0)\rangle = mk_BT\omega^{(2)}M_1(t)$. Here k_B, T, and m are the Boltzmann constant, the temperature, and the mass of a particle, respectively. Multiplying Eq. (1) by $v_\alpha(0)/\langle|v_\alpha(0)|^2\rangle$ and performing an appropriate ensemble average $\langle\ldots\rangle$, one obtains the memory equation for the VACF, i.e.:

$$\frac{da(t)}{dt} = -\omega^{(2)}\int_0^t M_1(\tau)a(t-\tau)d\tau, \qquad \langle v_\alpha(0)F(t)\rangle = 0; \quad (2)$$

here the VACF $a(t) = \langle v_\alpha(0)v_\alpha(t)\rangle/\langle v_\alpha(0)^2\rangle$ appears, which is related to the diffusion constant by the integral relation [13] $D = (k_BT/m)\int_0^\infty a(t)dt$.

Next we introduce a dimensionless parameter which characterizes memory effects for the relaxation process related to the velocity degree of freedom

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$$\delta = \frac{\tau_a^2}{\tau_M^2}, \tag{3}$$

$$\tau_a^2 = \left| \int_0^\infty t a(t) dt \right|, \qquad \tau_M^2 = \left| \int_0^\infty t M_1(t) dt \right|, \tag{4}$$

where τ_a^2 and τ_M^2 are the squared characteristic relaxation scales of the VACF and its corresponding memory function. Note that $0 \leq \delta < \infty$. Obviously, the situation $\tau_a^2 \gg \tau_M^2$ corresponds to a memoryless behavior with a fast-decaying memory. Then, in accordance with Eq. (3) we find that $\delta \to \infty$. For processes exhibiting strong, pronounced memory effects, $\tau_a^2 \ll \tau_M^2$, this parameter thus approaches $\delta \to 0$ [14].

Equation (4) can be rewritten in the terms of Laplace transforms of corresponding correlation functions, $\tilde{f}(z) = \int_0^\infty e^{-zt} f(t) dt$, in the following forms:

$$\tau_a^2 = \left| \lim_{z\to 0} \left(-\frac{\partial \tilde{a}(z)}{\partial z} \right) \right|, \qquad \tau_M^2 = \left| \lim_{z\to 0} \left(-\frac{\partial \tilde{M}_1(z)}{\partial z} \right) \right|. \tag{5}$$

After a Laplace transform, Eq. (2) reads:

$$\tilde{a}(z) = [z + \omega^{(2)} \tilde{M}_1(z)]^{-1}, \tag{6}$$

which allows one to obtain

$$-\tilde{M}_1'(z) = \frac{\tilde{a}'(z) + \tilde{a}(z)^2}{\omega^{(2)} \tilde{a}(z)^2}, \tag{7}$$

where $\tilde{a}'(z) = \partial \tilde{a}(z)/\partial z$ and $\tilde{M}_1'(z) = \partial \tilde{M}_1(z)/\partial z$. Then, taking into account the relations (5) we recast Eq. (3) as

$$\delta = \omega^{(2)} \left| \lim_{z\to 0} \frac{\tilde{a}'(z) \tilde{a}(z)^2}{\tilde{a}'(z) + \tilde{a}(z)^2} \right|. \tag{8}$$

Note that the knowledge of $a(t)$ and its first derivative at long times, i.e., for $z \to 0$, and $\omega^{(2)}$, is sufficient to evaluate the measure δ. The complete knowledge of the memory function is thus not required. Moreover, the frequency moment of the VACF $\omega^{(2)}$, and thus δ, is directly related to physical observable quantities such as the distribution function and the potential of interparticle interaction [15].

Let us consider two contrasting situations: (i) the system has a short-range memory, and (ii) the system is characterized by physical (long-range) memory.

In the first case (*the memory-free limit*) the memory function can be presented as $M_1(t) = 2\tau_1 \delta(t)$. Then Eq. (2) is reduced to the ordinary Langevin equation [16]:

$$m \frac{d}{dt} v_\alpha(t) + m\omega^{(2)} \tau_1 v_\alpha(t) = F(t) \tag{9}$$

with a simple exponential solution for VACF:

$$a(t) = e^{-\omega^{(2)} \tau_1 t}, \tag{10}$$

which is correct for the VACF of a free Brownian particle with the relaxation time $\tau_0 = (\omega^{(2)} \tau_1)^{-1} = m/\gamma$; m and γ are the mass and the friction coefficient, respectively. Let us define the parameter δ for this case. Applying the Laplace transform to the memory function and VACF [Eq. (10)] for this case, and taking into account Eq. (5) one can find that $\tau_a^2 = \tau_0^2$ and $\tau_M^2 = 0$. Then, Eq. (3) yields exactly $\delta \to \infty$.

The opposite situation is appropriate for systems that exhibit indefinitely large memory, i.e., the so-called *strong memory limit*. The time dependence for this model can be presented adequately as follows:

$$M_1(t) = H(t) = \begin{cases} 1, & t \geq 0 \\ 0, & t < 0 \end{cases}, \tag{11}$$

where $H(t)$ is the step Heaviside function. Introducing Eq. (11) into the convolution integral of Eq. (2), one obtains the following equation

$$\frac{da(t)}{dt} = -\omega^{(2)} \int_0^t a(\tau) d\tau,$$

which has the simple solution

$$a(t) = \cos(\sqrt{\omega^{(2)}} t). \tag{12}$$

The similar VACF describes oscillations of the lattice particles in crystalline solids. Using the Laplace transforms of Eqs. (11) and (12) we define from Eq. (5) the squares of characteristic relaxation scales of VACF and memory function, $\tau_a^2 = 1/\omega^{(2)}$ and $\tau_M^2 \to \infty$. Then, from definition (3) we find $\delta \to 0$. Thus, we have shown that the parameter δ possesses true meaning for both the memory-free and the manifest, strong memory limit.

We can therefore state with confidence that the quantity δ sensitively detects and measures the presence of memory effects. The offered measure of memory can be obtained theoretically, experimentally, and with the help of computer modeling if $\tilde{a}(z)$ [or $a(t)$] is known. We next evaluate δ for various model systems, thereby demonstrating its usefulness.

A. The Rubin model [17].—The particle impurity with the mass M is located in an infinite, 1D harmonic lattice, particles of which have the same mass m (K is the coupling constant). The crucial quantity here is the mass ratio $q = M/m \geq 1$. In case of $q \gg 1$ the movement of a particle with mass M is the same as the stochastic movement of a Brownian particle (the memory-free limit) [1]. If the mass ratio $q = 1$, then the system consists of particles of the same mass that correspond to the model for acoustic phonons in crystalline solids at ordinary temperatures (the strong memory limit) [18]. Thus, the Rubin model contains both memory-free and strong memory limits, transition to which is defined by value q. The term $\tilde{a}(z)$ and the frequency parameter $\omega^{(2)}$ have the following forms here [1]:

$$\tilde{a}(z) = \frac{q}{(q-1)z + \sqrt{z^2 + 4K/m}}, \qquad \omega^{(2)} = 2K/M. \tag{13}$$

From last expression we find

$$\tilde{a}(z=0) = q\sqrt{\frac{m}{4K}}, \qquad \tilde{a}'(z=0) = -\frac{M}{4K}(q-1). \tag{14}$$

Then, from Eq. (8) we find the expression

$$\delta = \frac{q}{2}|q-1|, \tag{15}$$

related δ with the quantity q. It is seen from the given relation that for the strong memory limit at $q = 1$ we have $\delta = 0$, and for the memory-free one we obtain $\delta \rightarrow \infty$. The squared q dependence in Eq. (15) defines the transition in this model from one limit to the other.

B. Ideal gas.—TCF of density fluctuations for an ideal gas [15] is

$$\phi(t) = \frac{\langle \rho(0)^* \rho(t) \rangle}{\langle |\rho(0)|^2 \rangle} = \exp(-\Omega_1^2 t^2/2). \tag{16}$$

Note that the Laplace transform of $\phi(t)$ is related to the Laplace transform of autocorrelator for a longitudinal component of velocity of local density fluctuations, $a_l(t)$, by

$$\tilde{\phi}(z) = [z + \Omega_1^2 \tilde{a}_l(z)]^{-1}. \tag{17}$$

The term $a_l(t)$ is similar to VACF and its frequency moment $\omega^{(2)}$ is related to Ω_1^2 by $\omega^{(2)} = 2\Omega_1^2$ [6]. Moreover, applying the Laplace transform to Eq. (16) and taking into account Eq. (17) one finds

$$\tilde{a}_l(z) = \sqrt{\frac{2}{\Omega_1^2 \pi}} \exp[-z^2/(2\Omega_1^2)] \operatorname{erfc}^{-1}\left(\frac{z}{\sqrt{2\Omega_1^2}}\right) - \frac{z}{\Omega_1^2}$$

with the following low-frequency properties

$$\lim_{z\to 0} \tilde{a}_l(z)^2 = \frac{2}{\pi\omega^{(2)}}, \qquad \lim_{z\to 0} \tilde{a}_l'(z) = \frac{2-\pi}{\pi\omega^{(2)}}. \tag{18}$$

Finally, one finds from Eq. (8) that

$$\delta = \frac{4(\pi - 2)}{\pi(4-\pi)} \approx 1.69. \tag{19}$$

It is evident that the relaxation process related to fluctuations of a longitudinal velocity (momentum) component in an ideal gas is characterized by pronounced memory and independent from model parameters such as $\omega^{(2)}$.

C. Interacting 2D electron gas at long wavelengths and at $T = 0$.—In Ref. [18] it was shown that TCF of density fluctuations and TCF of a longitudinal momentum component for this model are

$$\phi(t) = J_0(2\sqrt{\Omega_1^2} t), \qquad a_l(t) = \frac{J_1(2\sqrt{\Omega_1^2} t)}{\sqrt{\Omega_1^2} t}, \tag{20}$$

where $\Omega_1^2 = k^2 \epsilon_F^2$, ϵ_F^2 is the Fermi energy and k is measured in units of the Fermi vector k_F, J_n is the Bessel function of the nth order. It is necessary to note that in the case of such time dependence of $a_l(t)$, this TCF and its memory function have the same time behavior. As a result, they have the same relaxation time scales and $\delta = 1$ that is easily obtained by the Laplace transform of Eq. (20) with taking into account Eq. (8).

Long time tails.—As is known, TCF's in various physical systems can be characterized by long lasting tails [19]. For example, the long time behavior of VACF in liquids [1] is

$$\lim_{t\to\infty} a(t) \sim t^{-d/2}, \tag{21}$$

where $d = 2$ and 3 are two-dimensional and three-dimensional cases, correspondingly. In accordance with the Tauberian theorem, this is equivalent to

$$\lim_{z\to 0} \tilde{a}(z) \sim z^{d/2-1}. \tag{22}$$

Then, one obtains the following low-frequency properties

$$\begin{aligned} &\tilde{a}(z)^2 \sim 1, \qquad \tilde{a}'(z) = 0, \qquad \text{if } d = 2, \\ &\tilde{a}(z)^2 \sim z, \qquad \tilde{a}'(z) \sim \frac{1}{\sqrt{z}}, \qquad \text{if } d = 3, \end{aligned} \tag{23}$$

and from Eq. (8) we find that $\delta = 0$ for both cases. It is evident that the long time dynamics related to the fractal law (21) is characterized by memory effects which appear directly by conserved long-living correlations. From this point of view, the source of such behavior is in the presence of arbitrary fragments of the regular motion in the system dynamics likely to be found in the billiard model [20].

Anomalous diffusion.—Let us consider anomalous diffusion phenomena on an example of a free particle coupled to a fractal heat bath—the model used to study both sub- and superdiffusion. We do not consider the superdiffusion region including ballistic limit with $\alpha \geq 2$ [21]. The VACF for this model can be written as

$$a(t) = E_{2-\alpha}(-\gamma_\alpha t^{2-\alpha}), \qquad \gamma_\alpha = \frac{\pi A_0}{m k_B T \sin(\alpha\pi/2)}, \tag{24}$$

where $E_\alpha(t)$ is the Mittag-Leffler function and A_0 is the strength of the coupling [22]. Ordinary diffusion corresponds to $\alpha = 1$, superdiffusion is associated with motion at $1 < \alpha < 2$, while subdiffusion occurs when $0 < \alpha < 1$. Equation (24) for $\alpha \neq 1$ has an inverse power-law tail at long times [23]

$$a(t) \sim \frac{t^{\alpha-2}}{\gamma_\alpha}. \tag{25}$$

One can readily deduce that for subdiffusion with $\alpha < 1$ the parameter $\delta \rightarrow 0$. For example, at $\alpha = 1/2$ we obtain the same result as for a long time tail with $d = 3$ [see Eq. (23)]. Let us next consider superdiffusion with $1 <$

$\alpha < 2$. Then, for $\alpha = 3/2$ we have

$$\lim_{z\to 0} \tilde{a}(z)^2 \sim z^{-1}, \qquad \lim_{z\to 0} \tilde{a}'(z) \sim z^{-3/2}. \tag{26}$$

Taking into account Eq. (26) we find from Eq. (8) that $\delta \to \infty$. As a result, although the VACF behavior in this case strongly deviates from the exponential relaxation pattern, its memory function decays rather fast in comparison with the VACF; i.e., superdiffusion dynamics is similar to an ordinary Markovian process [24].

In conclusion, the notion of strong dynamical memory is rather characteristic for the statistical properties of the time evolution of many systems, and as demonstrated with our study it depends on physical features of the underlying process. From the point of view of a recurrent relation method, properties of memory can be associated with the topology of a Hilbert space, where a dynamical variable is represented as a vector [2]. Memory effects then occur both within a finite-dimensional space, and in an infinite-dimensional one, where the VACF is dissipative. On the basis of the GLE formalism we propose a convenient measure of memory effects in dynamical systems. This quantity is based on a definition that allows one to extract in a tractable manner the role of memory behavior for the dynamics, and moreover, allows one to test the validity of memory-free approximations. The simplicity of the given measure makes its application possible in the analysis of various complex systems. Although the role of memory effects for chaotic processes is not yet settled, the measure δ may provide a useful guide in establishing an interrelation of manifest memory for such fundamental properties as chaotic behavior [25] and ergodicity [26].

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