Relation between Anomalous and Normal Diffusion in Systems with Memory

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We present a simple criterion based on the Einstein relation for determining whether diffusion in systems governed by a generalized Langevin equation with long-range memory is normal, superdiffusive, or subdiffusive. We support our analysis with numerical simulations.

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Diffusion is one of the fundamental mechanisms for transport of materials almost everywhere in nature and has therefore been the focus of extensive research in many different disciplines of natural science. Many aspects of diffusion are, as a consequence, well understood today. However, open questions linger on, such as how the presence of correlated disorder in the medium where the diffusion takes place influences the diffusion process, possibly making it anomalously fast or slow. This particular question has prompted much research over the last couple of decades [1–3]. The disorder of the background medium may induce memory effect into the diffusion process, and it is the objective of this Letter to present an analysis of memory effects in diffusive systems. The analysis culminates in a simple criterion based on the structure of the memory function allowing us to determine whether the diffusion process is normal, i.e., described by a finite diffusion constant and spreading according to the standard diffusion constant, or whether the process is superdiffusive, and therefore having an infinite diffusion constant, or subdiffusive, which entails a vanishing diffusion constant. We demonstrate our analysis on an explicit example, and test it against numerical simulations.

Einstein derived a famous relation between the diffusion constant D, temperature T, and friction γ,

$$D = \frac{k_B T}{m\gamma}, \tag{1}$$

where m is the mass of the diffusing particle and k_B is the Boltzmann constant [4]. This relation is easily derived from a normal Langevin equation (NLE) of the form [5]

$$m\frac{d}{dt}v(t) + m\gamma v(t) = F(t), \tag{2}$$

where $v(t)$ is the velocity of the random walker and $F(t)$ an uncorrelated random force with properties $\langle F(t)\rangle = 0$ and $\langle F(0)F(t)\rangle = 2mk_B T\gamma\delta(t)$. The brackets $\langle\cdots\rangle$ indicate a thermal average. We now consider a disordered background medium. The disorder may occur in two ways. The background may have a fixed, disordered geometrical structure where long-range correlations may manifest themselves, for example, through the geometrical structure being fractal. Another way the background may be disordered is through temporal correlations in the interactions between the random walkers and the background. We consider in the following the second type of disorder. The NLE, Eq. (2), is then modified to a generalized Langevin equation (GLE) of Mori-Lee form [6,7],

$$m\frac{d}{dt}v(t) = -m\int_0^t \Gamma(t-t_1)v(t_1)dt_1 + F(t), \tag{3}$$

where the memory $\Gamma(t)$ is related to the stochastic force $F(t)$ through the fluctuation-dissipation theorem

$$C_F(t) = \langle F(t)F(0)\rangle = mk_B T\Gamma(t). \tag{4}$$

For short range memory $\Gamma(t) = 2\gamma\delta(t)$, Eq. (3) reduces to the NLE. For a system described by a GLE, the velocity correlation function $C_v(t) = \langle v(t)v(0)\rangle$ is a fundamental function from which it is possible to obtain the system's physical properties. In particular, Kubo obtained the diffusion constant as [8]

$$D = \lim_{t\to\infty}\frac{1}{2t}\langle x^2(t)\rangle = \int_0^\infty C_v(t)dt. \tag{5}$$

Here

$$\lim_{t\to\infty}\langle x^2(t)\rangle \propto t^\alpha \tag{6}$$

is the second moment of the position after the transient time. For $\alpha = 1$, we have normal diffusion and D is finite. For $\alpha < 1$, $D = 0$, and the motion is subdiffusive. Finally, for $\alpha > 1$, $D = \infty$, and the motion is superdiffusive.

Several authors have claimed that long-range correlations in the fluctuating force $F(t)$ may induce anomalous diffusion due to the absence of a time scale [2,3,9]. It is well known that long-range correlation functions may induce anomalous behavior, such as delayed fracture [10], or anomalous reaction rates [11], in addition to anomalous diffusion in disordered media. Such long-range correlations may even turn off the diffusion process for certain boundary conditions [12].

In this Letter we establish the conditions for a system described by Eq. (3) to present anomalous diffusion. We multiply Eq. (3) by $v(0)$ to perform an ensemble average. Since $\langle F(t)v(0)\rangle = 0$, we obtain

$$\frac{dC_v(t)}{dt} = -\int_0^t \Gamma(t-t_1)C_v(t_1)dt_1. \tag{7}$$

We Laplace transform this expression to obtain

$$\tilde{C}_v(z) = \frac{C_v(0)}{z+\tilde{\Gamma}(z)}, \tag{8}$$

where the tilde denotes the Laplace transform. The diffusion constant Eq. (5) is then given by

$$D = \tilde{C}_v(0) = \frac{C_v(0)}{\tilde{\Gamma}(0)}. \tag{9}$$

Consequently, it is enough to know $C_v(0)$ and $\tilde{\Gamma}(0)$ to determine the diffusion constant. Moreover, if $C_v(0)$ is finite, the diffusion process is controlled by $\tilde{\Gamma}(0)$.

Typically, a system that satisfies the equipartition theorem also satisfies the Einstein relation Eq. (1), where

$$\gamma = \tilde{\Gamma}(0) = \int_0^\infty \Gamma(t)dt \tag{10}$$

is the friction constant. Hence, if $\tilde{\Gamma}(0)$ is finite, the diffusion is the normal Einstein diffusion, and, consequently, it does not matter if the system has long time correlation or if the correlations are scale invariant. What does matter are the convergence properties of the integral (10).

We assume now that $\Gamma(t) \sim t^{-\beta}$, leading to

$$\tilde{\Gamma}(z) \sim z^{\beta-1}. \tag{11}$$

Since z plays the role of an inverse cutoff time scale in the Laplace transform,

$$\tilde{\Gamma}(z) = \int_0^\infty e^{-zt'}\Gamma(t')dt' \approx \int_0^{1/z}\Gamma(t')dt', \tag{12}$$

we see that

$$\tilde{\Gamma}(1/t) \sim t^{1-\beta}. \tag{13}$$

Hence, using Eq. (9), we find that $D = \lim_{t\to\infty} C_v(0)/\tilde{\Gamma}(1/t) \propto t^{\beta-1}$. Using Eqs. (5) and (6), we find that

$$\alpha = \beta. \tag{14}$$

Thus, knowing how $\Gamma(t)$ behaves as $t \to \infty$, or equivalently, how $\tilde{\Gamma}(z)$ behaves as $z \to 0$ determines α.

We now demonstrate these ideas on an explicit system. Consider a noise described by a bath of thermal oscillators of the form

$$F(t) = \int_0^\infty A(\omega)\cos[\omega t + \phi(\omega)]d\omega, \tag{15}$$

where $A(\omega)$ is obtained from the power spectrum. The random function $\phi(\omega)$, where $0 \le \phi(\omega) < 2\pi$, gives the stochastic character to the function $F(t)$. The system now has a fixed temperature T and a fluctuating energy; i.e., we are dealing with a canonical ensemble. The force correlation function is

$$C_F(t) = \langle F(t)F(0)\rangle = mk_BT\int_0^\infty \rho_n(\omega)\cos(\omega t)d\omega, \tag{16}$$

where $\rho_n(\omega) = A^2(\omega)/(2mk_BT)$ is the noise density of states (NDS) of the thermal bath. Let us note that Eq. (16) shows $C_F(t)$ to be an even function of t and that $\Gamma(t)$ is even as well. This result was pointed out by Lee for Hamiltonian (i.e., microcanonical) systems [13]. We have hence pointed out here the validity of this observation for a canonical system.

We can explore once more Eq. (9) if we rewrite

$$\gamma = \tilde{\Gamma}(0) = \lim_{z\to 0}\int_0^\infty \rho_n(\omega)\frac{z}{z^2+\omega^2}d\omega = \frac{\pi}{2}\rho_n(0). \tag{17}$$

Now we see that the NDS in the long-wavelength limit controls the diffusion. Note that it is necessary to know the NDS only to classify the diffusion process.

Consider the following NDS:

$$\rho_n(\omega) = \left\{\begin{array}{ll} C, & \text{for } \omega < \omega_S \\ 0, & \text{for } \omega > \omega_S \end{array}\right\}. \tag{18}$$

Here C is a constant. This corresponds, e.g., to the long-wavelength limit of one-dimensional acoustic phonons. For a noise originated from a coupled harmonic chain, ω_S is the Debye phonon frequency.

We calculate the memory function for this system and find

$$\Gamma(t) = \frac{2\gamma^*\omega_S}{\pi}\left(\frac{\sin(\omega_S t)}{\omega_S t}\right). \tag{19}$$

Using Eq. (10), we find that $\gamma = \gamma^*$. For superdiffusive systems, this relation may not hold; see Eq. (22). Note that this memory function has a t^{-1} behavior for large t. Laplace transforming Eq. (19) gives

$$\tilde{\Gamma}(z) = \frac{2\gamma^*}{\pi}\arctan\left(\frac{\omega_S}{z}\right). \tag{20}$$

Using Eqs. (11) and (14), we see that $\alpha = 1$; i.e., we have normal diffusion. Furthermore, we find the same diffusion constant as the NLE with friction $\tilde{\Gamma}(0) = \gamma$. Also, note that the limit $z \to 0$ in Eq. (20) is equivalent to the limit $\omega_S \to$

∞. However, $\omega_S \to \infty$ implies $\Gamma(t) = 2\gamma\delta(t)$, Eq. (3) reduces to the NLE, and, as expected, Eq. (9) reduces to the standard Einstein relation, Eq. (1). Rather than being a coincidence, this is a very general property.

We plot in Fig. 1 $C_v(t)$ here for $T = 0.08$, $\gamma^* = 0.25$, and $\omega_S = 0.5$ or 5, giving a ratio $\omega_S/\gamma^* = 2$ or 20, respectively. This measures the importance of the memory effects, which decreases with increasing ratio. Curves 1(a) and 1(b) have $\omega_S = 0.5$, while curve 1(d) has $\omega_S = 5$. Curve 1(a) shows numerical integration of Eq. (7), and curve 1(b) shows simulation of Eq. (3) using 1000 random walkers with independent sequences of noise. Curve 1(c) shows the behavior of a system without memory, while curve 1(d) shows simulation of Eq. (3). The oscillatory behavior for large t for the curves with small ratio is clear. Curve 1(d), with $\omega_S/\gamma^* = 20$, is, for all practical purposes, indistinguishable from $\omega_S \to \infty$. This is clear as curve 1(c) is based on an infinite ratio so that $C_v(t) = \exp(-\gamma^* t)$. There is a tremendous difference between curves (a), (b), (c), and (d) in Fig. 1, however, they all show the same normal diffusive behavior.

We now modify the NDS Eq. (18) by removing the lower part of the acoustic modes,

$$\rho_n(\omega) = \left\{ \begin{array}{ll} C, & \text{for } \omega_1 < \omega < \omega_S \\ 0, & \text{otherwise} \end{array} \right\}. \tag{21}$$

Here $\omega_1 < \omega_S$ is a finite frequency. This density of states yields

$$\Gamma(t) = \frac{2\gamma^*}{\pi}\left(\frac{\sin(\omega_S t)}{t} - \frac{\sin(\omega_1 t)}{t}\right). \tag{22}$$

We use now $\gamma^* = 0.25$, i.e., the same value used before. However, the reader should keep in mind that $\gamma^* \neq \gamma = 0$.

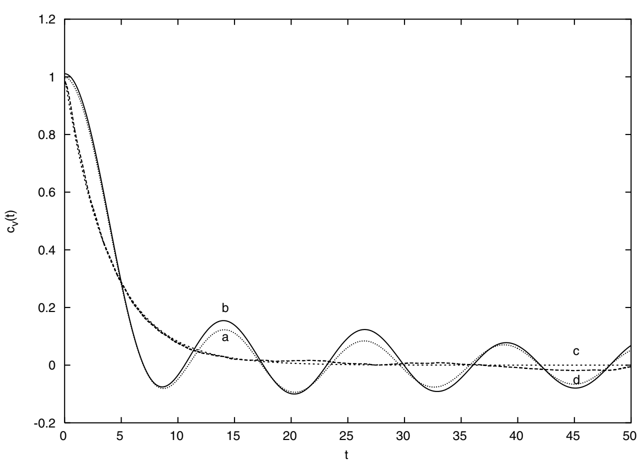

FIG. 1. $C_v(t)$ as a function of time t. We have set $T = 0.08$ and $\gamma^* = 0.25$. Curve (a) shows numerical integration of Eq. (7), and curve (b) shows simulation of the GLE using 1000 random walkers and independent sequences of noise. ω_S was set to 0.5. Curve (c) shows the behavior of a system without memory, while curve (d) shows simulation of the GLE for $\omega_S = 5$.

Now, considering Eqs. (9), (17), and (21), we predict that Eq. (22) shows superdiffusive behavior. In particular, for small z values, we find from Eq. (21) that $\tilde{\Gamma}(z) \propto z(1/\omega_1 - 1/\omega_S)$. Using Eqs. (11) and (14), we determine $\alpha = 2$ for this system.

In Fig. 2 we plot $\langle x^2(t)\rangle$ against t. The random walkers start from rest at the origin. Curve 2(a) shows the simulations of Eq. (3) with the NDS given by Eq. (18), using $\omega_S = 0.5$, while curve 2(b) shows the corresponding curve for the system without memory. In curve 2(c) we simulate Eq. (3) with the NDS given by Eq. (22), with $\omega_1 = \omega_S/2$; i.e., we exclude the lower half of the noise spectrum in such a way that $\rho_n(0) = 0$. The computer code used for the curves 2(a) and 2(c) is the same, except for the density range of frequencies. After the transient period all curves exhibit the behavior predicted by Eq. (6). Curves (a) and (b) in Fig. 2 show a straight line and hence $\alpha = 1$, with $D = 0.35$ and $D = 0.32$, respectively, which is very close to the exact value $D = 0.32$. Curve 2(c) shows a parabolic behavior with $\alpha = 1.98 \pm 0.01$, i.e., a superdiffusive behavior, as predicted above. $\alpha = 2$ is the limit for ballistic motion.

Now we return to our main variable, i.e., the velocity correlation function $C_v(t)$ that can be obtained as the inverse of the Laplace transform Eq. (8). Time reversal symmetry implies for $C_v(t)$ a relation similar to Eq. (16),

$$C_v(t) \sim \int_0^\infty \rho(\omega)\cos(\omega t)d\omega; \tag{23}$$

i.e., it can be associated with a Fourier transform with a density of states (DOS) $\rho(\omega)$. Equations (8) and (17) show that

$$\rho_n(\omega \simeq 0) \sim \rho^{-1}(\omega \simeq 0). \tag{24}$$

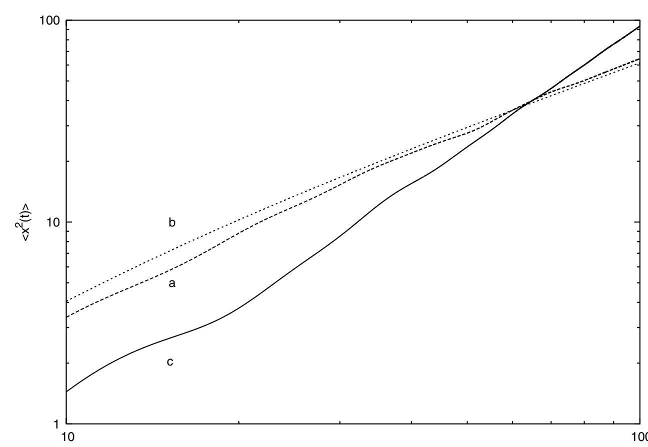

FIG. 2. $\langle x^2(t)\rangle$ vs t. Curve (a) shows a simulation of the GLE, with $\omega_S = 0.5$ and a NDS given in Eq. (18), while curve (b) is for the system without memory. Curve (c) shows a simulation of the GLE with a NDS given in Eq. (22), with $\omega_1 = \omega_S/2$. In this case we find superdiffusive behavior.

For the lowest modes, the DOS for the velocity correlation function is proportional to the inverse of the NDS. For example, Florencio and Lee [12] studied diffusion in a classical harmonic chain using a Hamiltonian formulation. They showed that the absence of the zero mode causes the diffusion constant to vanish. The equivalent of that in our case is an infinite NDS giving a zero value for Eq. (9).

So far we have obtained direct and clean results such as Eq. (17) which displays a relation between diffusive mechanisms and the NDS. Such a simple relation can be useful both theoretically and experimentally. We now address the rather controversial relation of this to experiments and consider spin diffusion in one-dimensional systems. Anderson, in his landmark paper [14], suggested the absence of spin diffusion in certain random lattices. On the other hand, the presence of low-temperature extended long-wavelength Goldstone modes in random magnets contradicts his conclusion [15]. Evangelou and Katsanos [16] have performed accurate numerical simulations for 1D lattices and showed the presence of superdiffusion associated with delocalization of the spin waves, i.e., a DOS of the form $\rho(\omega) \simeq \omega^{-\mu}$ $(0 < \mu < 1)$. Fluctuations in the density of states (FDS) decrease when the DOS increases [16]. Thus the classical NDS must be associated with the quantum fluctuations and, consequently, with the FDS which approaches zero for superdiffusion. From Moura *et al.* [17] data for FDS we get two regimes, $\mu \sim 0.5$ and $\mu \sim 1$, which from Eq. (11), $\mu = \alpha + 1$, allow us to predict $\alpha = 1.5$ and $\alpha = 2.0$ in perfect agreement with their results.

In conclusion, the results presented here are quite general and do not depend on complicated calculations or simulations. We showed that long-range memory does not necessarily imply anomalous diffusion. To classify the diffusion one need only know the quantity $\lim_{z\to 0} \tilde{\Gamma}(z)$. For systems described by a thermal bath generating harmonic noise, the NDS for the long-wavelength modes, $\rho(0)$, determines the process.

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