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NORMAL AND ANOMALOUS DIFFUSION: ERGODICITY AND FLUCTUATION–DISSIPATION THEOREM *

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We show a procedure for determining the class of diffusion in systems governed by a generalized Langevin equation with memory. The analysis holds for one-dimensional systems. We provide a simple answer for the diffusive exponent and its relation with noise and memory. We discuss as well limits for mixing, ergodicity and of the fluctuation–dissipation theorem.

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In this talk we shall address the problem of anomalous diffusion and its permanent presence in physics. This topic has been on for more than one hundred years and it still surprises us with new basic discoveries. Diffusion is one of the fundamental mechanisms for transport of materials, energy and information 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 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 [1, 2]. This particular question has prompted much research over the last couple of decades [1–7]. The disorder of the background medium may induce memory effect into the diffusion process, and our objective is 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

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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 start our analysis with the generalized Langevin equation (GLE) of Mori–Lee form [8–10],

$$m\frac{d}{dt}\,v(t) = -m\int\limits_0^t \Gamma(t-t_1)v(t_1)dt_1 + F(t)\,, \tag{1}$$

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

$$C_F(t) = \langle F(t)F(0)\rangle = mk_{\mathrm{B}}T\Gamma(t)\,. \tag{2}$$

For short range memory $\Gamma(t) = 2\gamma\delta(t)$, Eq. (1) reduces to the normal Langevin equation. 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 [11] obtained the diffusion constant as

$$D = \lim_{t\to\infty}\frac{1}{2t}\,\langle x^2(t)\rangle = \int\limits_0^\infty C_v(t)dt\,. \tag{3}$$

Here

$$\lim_{t\to\infty}\langle x^2(t)\rangle \propto t^\alpha\,, \tag{4}$$

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 induces anomalous diffusion due to the absence of a time scale (see [3, 4, 6, 7, 12]. and references therein). It is in addition well known that long range correlation functions may induce anomalous behavior, such as delayed fracture [13], or anomalous reaction rates [14] in addition to anomalous diffusion in disordered media. Such long-range correlations may even turn off the diffusion process for certain boundary conditions [15].

In this work we discuss the conditions for a system described by Eq. (1) to present anomalous diffusion [1–4]. We multiply Eq. (1) by $v(0)$ and to perform an ensemble average. Since $\langle F(t)v(0)\rangle = 0$, we obtain

$$\frac{dC_v(t)}{dt} = -\int\limits_0^t \Gamma(t-t_1)C_v(t_1)dt_1\,. \tag{5}$$

We Laplace transform this expression to obtain

$$\tilde{C}_v(z) = \frac{C_v(0)}{z + \widetilde{\Gamma}(z)}\,, \tag{6}$$

where tilde denotes the Laplace transform. The diffusion constant Eq. (3) is then given by

$$D = \tilde{C}_v(0) = \frac{C_v(0)}{\widetilde{\Gamma}(0)}\,. \tag{7}$$

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

Now, most of the physics will be described by the friction constant

$$\gamma = \widetilde{\Gamma}(0) = \int_0^\infty \Gamma(t) dt. \tag{8}$$

Hence, if $\widetilde{\Gamma}(0)$ is finite, the diffusion is the normal Einstein diffusion, and consequently it does not matter if the system has long time correlation nor if the correlations are scale invariant. What does matter are the convergence properties of the integral (8).

We assume now that

$$\widetilde{\Gamma}(z \to 0) \sim z^\beta\,, \tag{9}$$

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

$$\widetilde{\Gamma}(z) = \int_0^\infty \mathrm{e}^{-zt'} \Gamma(t') dt' \approx \int_0^{1/z} \Gamma(t')\ dt'\,, \tag{10}$$

we see that

$$\widetilde{\Gamma}(1/t) \sim t^{-\beta}\,. \tag{11}$$

Hence, using Eq. (7), we find that $D = \lim_{t\to\infty} C_v(0)/\widetilde{\Gamma}(1/t) \propto t^\beta$. Using Eqs. (3) and (4), we obtain

$$\alpha = \beta + 1\,. \tag{12}$$

Thus, knowing how $\Gamma(t)$ behaves as $t \to \infty$, or equivalently, how $\widetilde{\Gamma}(z)$ 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

$$F(t) = \int_0^\infty A(\omega) \cos(\omega t + \phi(\omega)) d\omega\,, \tag{13}$$

where $A(\omega)$ is obtained from the power spectrum. The random function $\phi(\omega)$ where $0 \leq \phi(\omega) < 2\pi$, 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

$$C_F(t) = \langle F(t)F(0)\rangle = mk_{\mathrm{B}}T \int_0^\infty \rho_n(\omega)\cos(\omega t)d\omega\,. \tag{14}$$

where $\rho_n(\omega) = A^2(\omega)/(2mk_{\mathrm{B}}T)$ is the noise density of states (NDS) of the thermal bath. We have used the relation $\langle\cos(\omega t + \phi(\omega))\cos(\omega' t + \phi(\omega'))\rangle = \delta(\omega - \omega')/2$. Let us note that Eq. (14) 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 [16]. We have hence pointed out here the validity of this observation for a canonical system.

We can explore once more Eq. (7) if we rewrite

$$\gamma = \widetilde{\Gamma}(0) = \lim_{z\to 0}\int_0^\infty \rho_n(\omega)\frac{z}{z^2+\omega^2}d\omega = \frac{\pi}{2}\rho_n(0). \tag{15}$$

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

Consider the following NDS

$$\rho_n(\omega) = \left\{ \begin{array}{lll} C, & \text{for} & \omega < \omega_S \\ 0, & \text{for} & \omega > \omega_S \end{array} \right\}. \tag{16}$$

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

$$\Gamma(t) = \frac{2\gamma^*\omega_S}{\pi}\left(\frac{\sin(\omega_S t)}{\omega_S t}\right). \tag{17}$$

Using Eq. (8), we find that $\gamma = \gamma^*$. For superdiffusive systems, this relation may not hold, see Eq. (20). Note that this memory function has a t^{-1} behavior for large t. Laplace transforming Eq. (17) gives

$$\widetilde{\Gamma}(z) = \frac{2\gamma^*}{\pi}\arctan\left(\frac{\omega_S}{z}\right). \tag{18}$$

Using Eqs. (9) and (12), we see that $\alpha = 1$, *i.e.*, we have normal diffusion. Furthermore, we find the same diffusion constant as the normal Langevin equation (NLE) with friction $\widetilde{\Gamma}(0) = \gamma$. Also, note that the limit $z \to 0$ in Eq. (18) is equivalent to the limit $\omega_S \to \infty$. However, $\omega_S \to \infty$ implies in $\Gamma(t) = 2\gamma\delta(t)$ and Eq. (1) reduces to the NLE, and as expected. Rather than being a coincidence, this is a very general property. For any time $t > 1/\omega_S$, the normal diffusion described by either GLE, or NLE, will lead to the same result. That is the reason we find a large number of phenomena where the diffusion is normal, even when we have strong correlations.

We now modify the NDS Eq. (16) by removing the lower part of the acoustic modes,

$$\rho_n(\omega) = \left\{ \begin{array}{ll} C, & \text{for} \quad \omega_1 < \omega < \omega_S \\ 0, & \text{otherwise} \end{array} \right\} . \tag{19}$$

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

$$\Gamma(t) = \frac{2\gamma^*}{\pi}\left(\frac{\sin(\omega_S t)}{t} - \frac{\sin(\omega_1 t)}{t}\right) . \tag{20}$$

We use now $\gamma^* = 0.25$, *i.e.* the same value used before. However, the reader should keep in mind that $\gamma^* \neq \gamma = 0$. Now, considering Eq. (7), (15), and (19), we predict that Eq. (20) shows superdiffusive behavior. In particular, for small z-values, we find from Eq. (19) that $\widetilde{\Gamma}(z) \propto z(1/\omega_1 - 1/\omega_S)$. Using Eq. (9) and (12), we determine $\alpha = 2$ for this system. Simulations confirms our result [1,17]. Those concept where used to generate a ratcher device [17].

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. (6). Time reversal symmetry implies for $C_v(t)$ a relation similar to Eq. (14)

$$C_v(t) \sim \int\limits_0^\infty \rho(\omega)\cos(\omega t)d\omega \, , \tag{21}$$

i.e. it can be associated to a Fourier transform with a density of states (DOS) $\rho(\omega)$. Equations (6) and (15) show that

$$\rho_n(\omega \simeq 0) \sim \rho^{-1}(\omega \simeq 0). \tag{22}$$

For the lowest modes, the DOS for the velocity correlation function is proportional to the inverse of the NDS. For example, Florencio and Lee [15] 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. (7).

Another important point is to know the limits where we can apply both GLE and the FDT. Recent results from Costa *et al.* [2] show that the FDT may fail for the ballist motion, $\alpha = 2$, and that seems to be a limit, for $\alpha > 2$ the stochastic description may not apply. The violation of the FDT is directly connect with the violation of mixing and ergodicit [16], which makes it an extremely important problem in physics with large applications on non linear dynamics [18].

In conclusion, the results presented here are quite general and do not depend on the specific form of the memory, the number of possible application is increasing and new results are expected. In particular a connection between the GLE and Hamiltonian systems have been recently formulated [19].

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REFERENCES

[1] R. Morgado, F.A. Oliveira, G.G. Batrouni, A. Hansen, *Phys Rev. Lett.* **89**, 100601 (2002).
[2] I.V.L. Costa, R. Morgado, M.V.B. Lima, F.A. Oliveira, *Europhys. Lett.* **63**, 173 (2003).
[3] F.A. Oliveira, R. Morgado, C. Dias, G.G. Batrouni, A. Hansen, *Phys. Rev. Lett.* **86**, 255839 (2001).
[4] F.A. Oliveira, R. Morgado, M.B.V.T. Lima, B.A. Mello, G.G. Batrouni, A. Hansen, *Phys. Rev. Lett.* **90**, 218901 (2003).
[5] J.P. Bouchaud, A. George, *Phys. Rep.* **195**, 127 (1990).
[6] H. Scher, M.F. Shlesinger, J.T. Bendler, *Physics Today* **44**, 26 (1991).
[7] M.F. Shlesinger, G.M. Zaslavsky, J. Klafter, *Nature* **363**, 31 (1993).
[8] R. Kubo, M. Toda, N. Hashitsume, *Statistical Physics II*, Springer Verlag, Berlin, 1998.
[9] H. Mori, *Prog. Theor. Phys.* **34**, 399 (1965).
[10] M.H. Lee, *Phys. Rev.* **B26**, 2547 (1982)
[11] R. Kubo, *Rep. Prog. Phys.* **29**, 255 (1966).
[12] T. Srokowski, *Phys. Rev. Lett.* **85**, 2232 (2000).
[13] F.A. Oliveira, *Phys. Rev.* **B57**, 10576 (1998).
[14] F.A. Oliveira, *Physica A* **257**, 128 (1998).
[15] J. Florencio, M.H. Lee, *Phys. Rev.* **A31**, 3231 (1985).
[16] M.H. Lee, *Phys. Rev. Lett.* **87**, 250601 (2001) .
[17] J.D. Bao, Y.Z. Huo, *Phys. Rev. Lett.* **91**, 138104 (2003).
[18] M.C. Ciesla, S.P. Dias, L. Longa, F.A. Oliveira, *Phys. Rev.* **E63**, 5202 (2001); L. Longa, E.M. Curado, F.A. Oliveira, *Phys. Rev.* **E54**, 2201 (1996).
[19] M.H. Vainstein, R. Morgado, F.A. Oliveira, F.A.B.F. de Moura, M.D. Coutinho-Filho, `cond-mat/0308542`.