Mixing, Ergodicity and slow relaxation phenomena

I.V.L. Costa, M.H. Vainstein, L.C. Lapas, A.A. Batista, F.A. Oliveira

ABSTRACT Investigations on diffusion in systems with memory [1] have established a hierarchical connection between mixing, ergodicity, and the fluctuation-dissipation theorem (FDT). This hierarchy means that ergodicity is a necessary condition for the validity of the FDT, and mixing is a necessary condition for ergodicity. In this work, we compare those results with recent investigations using the Lee recurrence relations method [2–4]. Lee shows that ergodicity is violated in the dynamics of the electron gas [4]. This reinforces both works and implies that the results of [1] are more general than the framework in which they were obtained. Some applications to slow relaxation phenomena are discussed.

Introduction – More than a hundred years after its formulation by Boltzmann, the ergodic hypothesis (EH) still drives the attention of the mathematics and physics community. Many situations have been found in which the EH is broken [1, 3–5]. On the other hand, the mixing condition (MC), despite being omnipresent in relaxation processes, has seldomly been the object of investigation [1, 6]. Recent studies on anomalous diffusion [1, 7] have established a strong hierarchy, which in growing generality is: the FDT, EH, and the MC. Since the FDT is a less general “theorem”, we shall focus only on the EH and the MC.

Kubo [8] realized that doing a time average on correlation functions would be more realistic than performing those averages on the variables themselves. He then established an ergodic condition in the framework of linear-response theory. That is, if the zero-frequency limit of a dynamical susceptibility is equal to its static counterpart, the system is ergodic. However, the problem of solving the dynamical equations of motion for many-body systems remains a daunting one at best, consequently the validation of the EH via Kubo’s method has been done only for a few systems.

With the development of the recurrence relations method by Lee [2], it became possible to obtain general solutions for the Heisenberg equations of motion. In this way it is possible to verify the validity of the EH [3, 4]. We have avoided this problem using the asymptotic limit of the correlation function, which allows us to verify the EH without a full solution of the dynamical equations of motion. For that, we just need the memory, which is our starting point. In this work we try to narrow the difference between the methods, i.e. we show that both methods yield the same result.

Ergodicity – Recently, Lee [4] proposed that the validation of the EH is subject to the
condition

\[ 0 < \tau = \int_0^\infty R(t) dt < \infty, \quad (1) \]

where \( \tau \) is a relaxation time we introduce here for further use, \( R(t) \) is the renormalized correlation function for the dynamical stochastic variable \( A(t) \). It is given by

\[ R(t) = \frac{\langle A(t)A(0) \rangle}{\langle A(0)^2 \rangle}, \quad (2) \]

and here \( \langle A(t)A(0) \rangle \) is the ensemble average. The finite value of the integral is the Lee condition \([4]\) for the EH be valid. Note that a necessary condition for the validity of Eq. \((1)\) is that the mixing condition \((MC)\) holds, i.e.

\[ \lim_{t \to \infty} R(t) = 0, \quad (3) \]

otherwise the integral would diverge. Consequently the MC is necessary for the EH, see Costa et al. \([1]\). The condition imposed by Lee is sufficient for the validity of the EH. However, there are situations where it may be too restrictive and this condition can be weakened. We shall prove here that in anomalous diffusion the MC is a sufficient condition.

Anomalous diffusion can be well described by a generalized Langevin equation (GLE) of the Mori form \([1, 7]\). From the GLE it is possible to obtain

\[ \frac{dR(t)}{dt} = -\int_0^t \Pi(t - t')R(t')dt', \quad (4) \]

where \( \Pi(t) \) is the memory. The Laplace transform of this equation yields

\[ \tilde{R}(z) = \frac{1}{z + \tilde{\Pi}(z)}, \quad (5) \]

where the tilde indicates Laplace transforms. Consider

\[ \lim_{t \to \infty} R(t) = \lim_{z \to 0} z\tilde{R}(z) = \lim_{z \to 0} \frac{z}{z + \tilde{\Pi}(z)}, \quad (6) \]

where we have used the final value theorem \([9]\). Note that the inverse Laplace transform can be obtained analytically only in a few cases. However, since we know \( \tilde{\Pi}(z) \) the limit can be obtained even without an explicit solution for \( R(t) \). For

\[ \tilde{\Pi}(z \to 0) \sim z^\nu, \quad (7) \]

the MC is not valid for \( \nu \geq 1 \). For diffusive processes with the mean-square displacement given by \( \langle x^2(t) \rangle \propto t^\alpha \), the exponent is \([1, 7]\) \( \alpha = \nu + 1 \). For \( \nu = -1 \) we have \( \alpha = 0 \), i.e. no diffusive process. This case needs special analysis: let \( \nu = -1 \), i.e. \( \tilde{\Gamma}(z) = K/z \). The inverse Laplace transform gives \( \Gamma(t) = K \). A constant value will produce a harmonic oscillator term which localizes the particle, i.e. no diffusion, in agreement with \( \alpha = \nu + 1 \).

From Eq. \((5)\), we get that \( R(t) = \cos(\sqrt{K}t) \). We can see that this correlation function
has an infinite relaxation time, and violates the MC and EH. Consequently, mixing and ergodicity in diffusive processes will hold only for $-1 < \nu < 1$, which correspond to $0 < \alpha < 2$. For $\nu = 0$ (normal diffusion), we can define a finite relaxation time by Eq. (11). Strictly speaking, one can define a relaxation time only for normal diffusion. In that case, with broad-band noise, the correlation function relaxes as $\exp(-t/\tau)$ [10]. We shall analyze here the extreme cases where the MC condition is violated.

**Slow Relaxation Phenomena** – We shall restrict ourselves to diffusive phenomena in order to compare our results with those of Lee. The majority of systems that violate ergodicity present some form of slow dynamics. For example Mukamel et al. [5] show that Ising systems with long-range interactions exhibit a relaxation time which diverges logarithmically with system size.

Another example of violation of the MC, which again implies the violation of the EH, is the ballistic motion, which we shall discuss in the next section. Let us now address the superdiffusive motion i.e. $0 < \nu < 1$.

As we have mentioned before, relaxation times exist only for normal diffusion. However, for superdiffusion, Eq. (4) in the limit given by Eq. (7), yields a Mittag-Leffler function of the form $E_{1-\nu}(-(t/\tau_\nu)^{1-\nu})$, which displays a transient behavior from a stretched exponential $\exp\left[-(t/\tau_\nu)^{1-\nu}\right]$ to a power law $(t/\tau_{\nu-1})^{\nu-1}$. In order to have an idea of the magnitude of $\tau$, we need to know the behaviour of $\tilde{\Pi}(z)$ for small $z$. This depends on the nature of the noise in the stochastic process [6] For a noise density of the form

$$\rho(\omega) = \begin{cases} 2\gamma \pi \frac{\omega}{\omega_D}^{\nu}, & \text{if } \omega < \omega_D \\ 0, & \text{otherwise}, \end{cases}$$

(8)

with $\omega_D$ as a Debye cutoff frequency, it is possible to compute the memory [1, 7] using the Laplace transform, and its low $z$ limit, to obtain the coefficient of Eq. (7). The transient time is $\tau_\nu = \tau_0 \left[(\gamma/\omega_D)^{\nu} \sec\left((\nu\pi)/2\right)^{1/(\nu-1)}\right]$. In Fig. 1 we plot the transient time $\tau_\nu$ as a function of $\nu$ for several values of $\omega_D/\gamma$. For normal diffusion, $t_0 = 1/\gamma$, it is equivalent to the relaxation time. Notice that the maximum increases with $\omega_D/\gamma$. For broadband noise $\omega_D/\gamma \gg 1$, the transient time becomes very large as $\nu$ approaches 1.

**Ballistic Motion** – In nature, normal diffusion and subdiffusion are prevalent, as can be observed in most conductors [11]. However, very recently in the history of conductivity investigations, superdiffusive and even ballistic motion have been produced in laboratories. This introduces a new and important field of investigation [12–17]. Indeed, we can find reliable reports on ballistic conductivity in carbon nanotubes [12, 13], in semiconductors [18], and in semiconductor superlattices with intentionally-correlated disorder [14,15]. We discuss here the violation of MH and EH in ballistic motion.

For ballistic conduction $\tilde{\Pi}(z) \propto cz$, where $c$ is a number without dimensions. The limit becomes

$$\lim_{t \to \infty} R(t) = (1+c)^{-1} \neq 0,$$

(9)

and the MC is violated. This implies that the EH and the FDT are violated [1].
Briefly, for some processes like anomalous diffusion the Lee condition Eq. (1) for the EH is too restrictive and in order to have the EH, we need only the MC. Moreover, the integral is finite only for normal diffusion, $\alpha = 1$. For anomalous diffusion in the range $0 < \alpha < 2$, the integral is either null ($0 < \alpha < 1$) or infinite ($1 < \alpha < 2$). In all these cases, the MC, the EH and the FDT are valid. At the extreme limit $\nu = -1$, or $\alpha = 0$, the system behaves as a localized harmonic oscillator and violates the MC, the EH and the FDT; for $\alpha = 2$, ballistic motion, the system also violates MC, and consequently the EH, and the FDT fail.

**Conclusion** – In this work we revisited the problem of the validity of the EH and that of the MC, and we obtained an agreement between our previous result [1] and recent results using the recurrence relations method [4]. However, for anomalous diffusion our condition can be less restrictive than that of Lee. Since diffusion is a main phenomenon in physics we use that as our starting point. The method used by Lee [2–4] is quite general and applies to any response function. In this context, the equivalence between this and our results strengthens both. The violation of the EH is exhibited for ballistic and harmonic motions. We have not focused deeper on real complex systems; we chose to follow easy-to-understand concepts where limits can be analytically obtained. This gave us a good framework for analyzing more complex structures. Nonlinear dynamics is a field which deserves much attention; in particular, the coalescence of trajectories has been intensively studied in the last few years [19–21]. The restriction of the degrees of freedom there may confirm the hierarchy exposed here. We also expect that new mathematical methods [22] may bring alternative proofs to the problem.

**Acknowledgments** – We thank professor Howard Lee for letting us read his manuscript prior to publication. This work was supported by the Brazilian agencies: CAPES, CNPq, FINEP, and FINATEC.
References

[1] I. V. L. Costa, R. Morgado, M. V. B. T. Lima, and F. A. Oliveira. Europhys. Lett., 63:173, 2003.

[2] M. H. Lee. Phys. Rev. B, 26:1072, 1982.

[3] M. H. Lee. Phys. Rev. Lett., 87:250601, 2001.

[4] M. H. Lee. J. Phys. A: Math. Gen., 39:4651, 2006.

[5] D. Mukamel D, S. Ruffo, and N. Schreiber. Phys. Rev. Lett., 95:240604, 2005.

[6] M. H. Vainstein, I. V. L. Costa, and F. A. Oliveira. Lecture Notes in Physics, 688:159 (2006), cond-mat/0501448.

[7] R. Morgado, F. A. Oliveira, G. G. Batrouni, and A. Hansen. Phys. Rev. Lett., 89:100601, 2002.

[8] R. Kubo, M. Yokota, and S. Nakajima. J. Phys. Soc. Jpn., 12:570–586, 1957.

[9] M. R. Spiegel. Theory and Problems of Laplace Transforms. McGraw-Hill, New York, 1965.

[10] M. H. Vainstein, I. V. L. Costa, R. Morgado, and F. A. Oliveira. Europhys. Lett., 73:726, 2006.

[11] J. C. Dyre and T. B. Schroder. Rev. Mod. Phys., 72:873, 2000.

[12] S. Frank, P. Poncharal, Z. L. Wang, and W. A. de Heer. Science, 280:1744, 1998.

[13] P. Poncharal, C. Berger, Y. Yi, Z. L. Wang, and W. A. de Heer. J. Phys. Chem. B, 106:12104, 2002.

[14] V. Bellani, E. Diez, R. Hey, L. Toni, L. Tarricone, G. B. Parravicini, F. Domínguez-Adame, and R. Gómez-Alcalá. Phys. Rev. Lett., 82:2159, 1999.

[15] V. Bellani, E. Diez, A. Parisini, L. Tarricone, R. Hey, G. B. Parravicini, and F. Domínguez-Adame. Physica E, 7:823, 2000.

[16] F. A. Oliveira, R. Morgado, A. Hansen, and J. M. Rubi. Physica A, 357:115–121, 2005.

[17] M. H. Vainstein, R. Morgado, F. A. Oliveira, F. A. B. F. de Moura, and M. D. Coutinho-Filho. Phys. Lett. A, 339:33–38, 2003.

[18] B. B. Hu, E. A. de Souza, W. H. Knox, J. E. Cunningham, M. C. Nuss, A. V. Kuznetsov, and S. L. Chuang. Phys. Rev. Lett., 74:1689–1692, 1995.

[19] L. Longa, E. M. F. Curado, and F. A. Oliveira. Phys. Rev. E, 54:R2201, 1996.

[20] M. Ciesla, S. P. Dias, L. Longa, and F. A. Oliveira. Phys. Rev. E, 63:065202(R), 2001.

[21] S. Boccaletti, J. Kurths, G. Osipov, D. L. Valladares, and C. S. Zhou. Phys. Rep., 366:1–101, 2002.
[22] C. C. Y. Dorea, A. V. Medino. *J. Stat. Phys.*, 123:685–698, 2006. doi:10.1007/s10955-006-9074-2.