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Editorial: The Fluctuation-Dissipation Theorem Today

Ewa Gudowska-Nowak[1], Fernando A. Oliveira[2,3] and Horacio Sergio Wio[4]*

[1]Institute of Theoretical Physics, Jagiellonian University, Kraków, Poland, [2]Instituto de Física, Universidade de Brasília, Brasília, Brazil, [3]Instituto de Física, Universidade Federal da Bahia, Campus Universitário da Federação, Salvador, Brazil, [4]Institute of Interdisciplinary Physics and Complex Systems, UIB-CSIC, Palma de Mallorca, Spain

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Editorial on the Research Topic

The Fluctuation-Dissipation Theorem Today

The concept of FDT is rooted in analysis of response relations appearing in systems subject to stimuli and driven away from equilibrium. In a linear response regime, close to equilibrium, use of Onsager's reciprocity relations [1] allows to calculate transport coefficients (see a following didactic review by Maes, this volume). Another form of response refers to the Einstein-Smoluchowski relation [2–5] between the coefficient of diffusion and the mobility, derived for a free Brownian particle in a fluid environment. At the level of Langevin equation [6] this result can be further rephrased as the relation between inverse of mobility and autocorrelation of the fluctuating force experienced by the Brownian particle. In his seminal works Onsager [1] demonstrated that symmetries in the susceptibility (response functions) were associated with the crystal symmetry. Later the quantum formula of FDT was given by Callen and Welton [7] who extended the Nyquist relation for the voltage fluctuations in electrical impedances of conductors. Advancements by Mori generalized the Langevin equation to include quantum effects and memory, next Kubo obtained the proper FDT for the Mori equation [8–10] Reggiani and Alfinito. Those historical series of results grounded the theory of relaxation of macroscopic perturbations and dynamics of fluctuations in systems around equilibrium.

Further developments in fluctuation-dissipation theory addressed the issue of interesting non-equilibrium phenomena—like slow relaxing structural glasses and proteins, mesoscopic radiative heat transfer or driven granular media where the violation of FDT was observed [11–18]. For growth phenomena such as those described by the Kadar-Parisi-Zhang equation [19] different formulations of the FDT have been proposed [20, 21]. Yet another approach has been put forward to investigate fluctuation-dissipation relation in systems exhibiting anomalous transport properties, including sub- and super-diffusion [22, 23].

The contents of this special topic devoted to FDT and applications is organized as follows: The article by Maes features derivation of response relations stemming from a trajectory-based description. Author presents an approach based on dynamical ensembles determined by an action on trajectory space and reviews fluctuation-dissipation relations of the first and second kind. Notion on active particles, where local detailed balance does not hold is reviewed, along with a discussion of open problems pertinent to response around nonequilibrium states. Within the article the concept of frenesy (or dynamical activity) as a complement to entropy in systems acting far from equilibrium is revisited [24]. Frenesy, defined as the time-symmetric part of the path-space action measuring difference between activated traffic and the path-wise escape, plays a crucial role in understanding selection of occupation and current statistics in systems with broken time-reversal symmetry. The excess in dynamical activity is proposed as a new Lyapunov functional.

Next, in the article *Beyond the Formulations of the Fluctuation Dissipation Theorem Given by Callen and Welton (1951) and Expanded by Kubo (1966)* Reggiani and Alfinito discuss the quantum

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Alex Hansen,
Norwegian University of Science and Technology, Norway

****Correspondence:***
Fernando A. Oliveira
faooliveira@gmail.com

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FDT and some challenges associated with it. The zero point contribution that is present in the quantum formulation of FDT as given by Callen-Welton and Kubo is known to lead to the so called vacuum catastrophe (it produces an ultraviolet catastrophe of the noise power spectral density). They propose a solution to this challenge by taking into account the Casimir energy [17] that, in turn, is found to be responsible for a quantum correction of the Stefan-Boltzmann law Reggiani and Alfinito, [25].

Florencio and Bonfim in *Recent Advances in the Calculation of Dynamical Correlation Functions* review some theoretical methods that have been used to calculate dynamical correlation functions of many-body systems. Time-dependent correlation functions and their associated frequency spectral densities are the quantities of interest, since they are fundamental to understanding both the theoretical and experimental dynamic properties. In particular, dynamic correlation functions appear in the FDT, where the response of a many-body system to an external perturbation is given in terms of the relaxation function of the unperturbed system, provided the disturbance is small. The method of recurrence relation has, at its foundation, the solution of Heisenberg equation of motion of an operator in a many-body interacting system [10]. The approach based on recurrence relations has been used in quantum systems such as dense electron gas, transverse Ising model, Heisenberg model, XY model, Heisenberg model with Dzyaloshinskii-Moriya interactions, as well as for classical harmonic oscillator chains. Effects of disorder have been considered in some of those systems. In the cases where analytical solutions were not feasible, approximation schemes have been used, although they have shown to be highly model-dependent.

Precise determination of diffusive properties for a system described by the generalized Langevin equation is discussed in *Time-dependent Fractional Diffusion and Friction Functions for Anomalous Diffusion* by Bao. The time-dependent fractional diffusion function and Green-Kubo relation, as well as the generalized Stokes-Einstein formula, in the spirit of ensemble averages, are reconfigured. The effective friction function is introduced as a measure of the influence of a frequency-dependent friction on the evolution of the system. Ergodicity is discussed from genaralization of the Debye model. Some results of the literature are critically reviewed.

In the work Chen *Application of the Brown Dynamics Fluctuation-Dissipation Theorem to the Study of Plasmodium berghei Transporter Protein PbAQP*, Chen gives an example of application of the FDT in biology. There he study the parasite *Plasmodium berghei (Pb)*, which causes diseases, *via* the investigation of the fluctuations in the transport across the membrane of neutral solutes. This is explicted *via* a Brownian dynamics fluctuation-dissipation theorem (BD-FDT). Laboratory mice infected by *Pb* exhibit symptoms that are equivalent to human malaria Bao caused by *Plasmodium falciparum (Pf)*. The parasite *Pb* has been used as basic organism to investigate the human malaria, mainly due to the simplicity of its genetic engineering. The investigation of the flux of water, glycerol and the wastes of used material, across the cell membrane, give us a good example of application of the FDT. In addition to the results exposed in his investigation, an analysis of the method developed there suggest that it is general and can be applied in similar situations. i.e., in the transport of neutral material across membranes of another parasites.

The article *Characterizing the Non-equilibrium Dynamics of Field-Driven Correlated Quantum Systems*, by Fotso and Freericks reviews recent studies on non-equilibrium dynamical mean-field theory (DMFT) of both transient and steady states of a DC field-driven correlated quantum system. They have shown that for an isolated system the relaxation to a steady state satisfying the fluctuation-dissipation theorem can be observed. The monotonic thermalization scenario is analyzed with the system monotonically approaching an infinite temperature thermal state (satisfyng the FDT) evolving through a series of consecutive quasi-thermal states satisfying the FDT only approximately. Focusing on the DMFT for the Falicov-Kimball model, they describe a Fermi-Fermi mixture of heavy and light particles, driven away from equilibrium by a constant electric field, showing a complex range of relaxation behaviors. For instance, the density of states shows the formation of Wannier-Stark ladders and the dielectric breakdown arising in presence of mid-gap states, absent in equilibrium. Authors describe also emergence of some key timescales in the current, manifested in the Wigner distribution function and its evolution towards infinite temperature. Their results illustrate the rich physics behind field-driven correlated quantum systems and the role that FDT plays in understanding of such behavior.

In *Generalized Fluctuation-Dissipation Theorem for Non-equilibrium Spatially Extended Systems* Wu and Wang have established a generalized form of the FDT for spatially extended non equilibrium stochastic systems described by continuous fields. Such a generalized FDT is formulated exploiting the non-equilibrium force decomposition in the potential landscape and flux field theoretical framework. Through concrete studies they support and validated the generalized FDT. Among others, a feature worth to be highlighted is that this generalized FDT represents a ternary relation at variance with the binary one arising in the equilibrium case. That is, in addition to the field correlation and the response function, existing in the equilibrium FDT, an additional flux correlation, entering into the FDT and qualitatively altering its structure, transforms it into a ternary relation.

Another article in this volume by Feng and Wang tackles the problem of non-equilibrium quantum systems characterized by detailed balance breaking. By using coherent phase space representation in quantum mechanics, the authors derive the gauge field and internal curvature to a generic class of non-equilibrium bosonic quantum systems coupled with the environments. It is shown that the internal curvature of the derived gauge field provides a direct measure of detailed balance breaking for non-equilibrium quantum systems. Moreover, it delivers a new, geometric view for the general nature and behaviors of non-equilibrium quantum systems, such as the fluctuation-dissipation theorem (FDT).

It is quite clear that after one hundred years the FDT still remains a central result and a major theorem in statistical physics, with many different formulations in classical and quantum theories. Two distinct aspects of the FTD are pursued: On the one hand, the theorem is of great practical importance because it establishes the relationship between susceptibilities; i.e., responses of the system Florencio and Bonfim, Bao, Chen to the perturbation field and correlations of physical observables measured in the reference unperturbed state. On the other, the FDT is closely connected to some basic principles in statistical mechanics such as ergodicity breaking and the Khinchin theorem [10, 26]. The standard form of FDT applies only to weak perturbations, close to thermal equilibrium states. However, over the past years a great effort has been made to generalize the FDT to classical systems far from equilibrium and to quantum systems, where FDT proved useful to study multipartite entanglements of complex quantum systems [27].

As an example, the FDT does not work in the KPZ equation for higher dimensions. This observation became an impediment to determining the KPZ exponents. Recently Anjos et al. [28] proposed that the growth dynamics builds up an interface with a fractal dimension d_f, which filters the original fluctuations given origin to new fluctuations which, by it turns, yields a new FDT in the fractal space. This allows a possible solution for the KPZ exponents [29]. There is much hope that this approach will drive us to unexpected hidden symmetries and new formulations of the FDT, in line with a visionary comment expressed by Giorio Parisi in *the year of physics concept* [30]. Last but not least, it is important to mention that Giorgio Parisi was awarded the Nobel Prize in Physics 2021 "for the discovery of the interplay of disorder and fluctuations in physical systems from atomic to planetary scales" [31].

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