Introduction to Focus Issue: Linear response theory: Potentials and limits

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Linear response theory (LRT) constitutes a cornerstone of statistical mechanics. Developed in the 1960s for thermostatted Hamiltonian systems, applications now include modern areas of research such as neurodynamics and climate science. If a system has linear response, one can estimate the change of expectation values caused by a perturbation using only information of the unperturbed system. LRT has been successfully applied for many dynamical systems in a predictive mode to determine their response to prescribed perturbations in the realistic case when the equilibrium density is not known. LRT also found its way into science as a tool to design and calibrate model reductions of high-dimensional complex systems. Almost independently from these success stories in applying LRT to understanding and controlling the natural world, mathematicians studied the dynamical ingredients necessary in a system to assure its linear response behavior, and found that many simple dynamical systems actually fail to obey LRT. Understanding, applying, and developing LRT remains an exciting and important endeavor. This Focus Issue brings together physicists and mathematicians from several areas to provide a state-of-the-art perspective.

I. INTRODUCTION

Since its introduction in the 1960s, linear response theory (LRT) has enjoyed a wide applicability across numerous disciplines to quantify the change of the mean behavior of observables when subjected to a perturbed environment.[1–3] LRT relies on the invariant measure being differentiable with respect to the perturbation. If this is the case, it allows us to express the average of an observable when subjected to small perturbations from an unperturbed state—the system's so-called *response*—entirely in terms of the invariant measure of the unperturbed system. Hence, the average behavior of a perturbed system can be determined using only information of the current unperturbed state of the system. In the context of climate science, the average observable may be global mean temperature and the perturbation may be an increase in greenhouse gas emission.

LRT has received increasing interest in the past decade. This interest has been spawned by successful applications in new areas such as neurophysiology and climate science,[4–7] as well as by surprising results in mathematics about the (non)validity of LRT in simple systems.[8–11] This Focus Issue compiles a gamut of reviews and original contributions to highlight the wide applicability in understanding and controlling the natural world as well as in uncovering fundamental mechanisms in the overall statistical behavior of complex dynamical systems. The contributions of this Focus Issue point toward numerous new avenues in which LRT can be used outside the typical realm of equilibrium statistical physics and invite us to engage with this powerful and remarkable theory.

II. SUMMARY OF CONTRIBUTIONS

Comprehensive reviews on how linear response theory contributes to our understanding of the natural world are provided by Sarracino and Vulpiani[12] and by Cessac.[13] Sarracino and Vulpiani[12] show how fluctuation dissipation relations can be deduced for a plethora of nonequilibrium systems including dissipative chaotic systems, multiscale systems, driven granular media, active particles, and systems exhibiting anomalous transport. The authors establish that for nonequilibrium systems, the correlations between numerous degrees of freedom may become important and that fluctuation dissipation relations based on marginal distributions are typically bound to fail for such systems.

Cessac[13] reviews recent advances in how LRT can be used in neurophysiology to understand the effect of external stimuli on the dynamics of networks of neurons, in particular, on collective behavior in the Amari–Wilson–Cowan model and in Integrate and Fire models.[13] Contrary to thermostatted Hamiltonian systems for which LRT was initially conceived, in neural dynamics, there is no conserved energy and the equilibrium dynamics is not time-reversible. Cessac shows that, nevertheless, a Gibbs distribution can be defined, allowing us to study linear response of systems of neurons. Interestingly, resonances of the susceptibility functions have neurophysiological interpretations.

Linear response theory is now a tool, used in contexts outside of equilibrium statistical mechanics. In this Issue, Maes and Netočný[14] employ linear response theory to gain understanding of how path-dependent nongradient forces may occur for a probe when coupled to a nonequilibrium environment. They find that the nonequilibrium environment generates a rotational force which by using linear response theory can be expressed in terms of the entropy flux and the frenesy of the nonequilibrium environment. Interestingly, the authors find that rotational components of the induced force appear if the frenesy has a nonvanishing projection orthogonal to the entropy flux.

Zhang *et al.*[15] use linear response theory and fluctuation dissipation theory to devise a numerical method for a reliable estimation of the drift and diffusion parameters obtained from time series of systems that can be described by stochastic differential equations. The authors estimate these parameters by solving a dynamic-constrained least-squares problem. The proposed method minimizes the difference between the linear response operator obtained from the time series and obtained from a stochastic differential equation whose drift and diffusion terms are to be determined. By judiciously designing a polynomial surrogate model for the cost function and assuming the knowledge of the equilibrium density of the system, the authors design a computationally cheap algorithm to reliably estimate the parameters of the stochastic diffusion dynamics. This may have interesting applications in molecular dynamics.

Abramov extends the notion of linear response formulas to the situation of impact perturbations of finite amplitude in which the state variables are perturbed at one instance of time by an arbitrary large magnitude, and then after the impact perturbation evolve again according to the unperturbed dynamics.[16] Explicit formulas are derived for the average response in several situations. Both deterministic impact perturbations and perturbations in which the magnitude and the time of impact are randomly drawn from independent distributions are being considered. In the latter case, the average linear response formula is an approximation, and it is argued that its accuracy is good provided the times between subsequent impacts are sufficiently small compared to the intrinsic time of decay of correlation of the dynamical system. The response formulas for such impact perturbations are nonlinear in the perturbation, prohibiting the estimation of the applied perturbation from an observed response.

Majda and Qi's contribution[17] also addresses the limitation of classical linear response theory to small perturbations. They review their results on how to employ linear and nonlinear response theory for complex turbulent systems and illustrate them with numerical simulations of several dynamical systems with varying complexity. Examples are given where despite a near-Gaussian probability function, a quasi-Gaussian closure leads to good predictions of the linear response of the mean but leads to wrong predictions of the linear response for the variance. The authors design reduced stochastic models, the parameters of which are calibrated to minimize an information-theoretic metric measuring the distance between the respective response operators of the imperfect model and the truth. The reduced stochastic models are shown to describe the response of the mean and of higher order moments well and are able to predict extreme events. The authors further illustrate how linear response theory can be used to determine the optimal control needed to drive a system back to some specified equilibrium state.

The problem of driving a system back to a prescribed state has particular relevance for climate change. Bódai *et al.* shed a critical light on using linear response theory to determine and to assess the effect of possible geoengineering strategies.[18] Using a climate model of intermediate complexity, the authors present the simulated response to a geoengineering scenario under an idealized greenhouse gas emission scenario and compare it with the response obtained via LRT, where the geoengineering is determined to achieve a desired constant global mean temperature. The results suggest that issues such as the sensitivity of the estimated response to the knowledge of the susceptibility function as well as possible higher-order nonlinear responses may leave LRT as insufficient to determine the required geoengineering and to assess geoengineering strategies. In particular, the authors give some indication that the uncontrolled response under geoengineering is typically more nonlinear for regional precipitation than for regional temperature in the studied model.

Ever since the work of Baladi and co-workers, who showed that simple dynamical systems such as the logistic map do not obey linear response, mathematicians have tried to develop frameworks to study if linear response exists for certain classes of dynamical systems. Galatolo and Sedro[19] develop such a framework based on transfer operators. They introduce a suite of assumptions such that linear and quadratic response can be guaranteed. The authors consider both deterministic and random dynamical systems with additive noise. In the latter case, they consider the so-called annealed case where, in addition to the ensemble average, an average with respect to the random parameters is taken. They find that in the additive noise case, linear and quadratic response exists even for systems without hyperbolicity. Two core assumptions are the existence of some resolvent of the unperturbed transfer operator and that the unperturbed dynamics is mixing (without restrictions on the mixing rate).

Castro[20] addresses LRT in the framework of transfer operators and the thermodynamic formalism for nonuniformly dynamics, including intermittent maps. The challenge when using transfer operators is to define Banach spaces, which allow for a spectral gap. Employing anisotropic spaces, the author shows the existence of statistical limit theorems, the statistical stability of the transfer operator, and the differentiability of thermodynamic quantities for nonuniformly expanding maps.

Wormell and Gottwald[21] ask the question of how linear response of macroscopic observables may be found in high-dimensional deterministic systems made up of mean-field coupled microscopic subunits, which individually may not obey linear response theory. They provide a comprehensive analysis of linear response behavior for both finite systems and for their thermodynamic limit. They find that such high-dimensional systems satisfy linear response if the macroscopic dynamics exhibits effective stochastic behavior via self-generated noise and if the distribution of the microscopic parameters is appropriately smooth. Maybe surprisingly, they also provide an example of a high-dimensional mean-field coupled system that violates LRT despite all microscopic subsystems having linear response.

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REFERENCES

[1] R. Kubo, "Statistical-mechanical theory of irreversible processes. I. General theory and simple applications to magnetic and conduction problems," J. Phys. Soc. Jpn. **12**, 570–586 (1957).

[2] R. Kubo, M. Yokota, and S. Nakajima, "Statistical-mechanical theory of irreversible processes. II. Response to thermal disturbance," J. Phys. Soc. Jpn. **12**, 1203–1211 (1957).

[3] R. Kubo, "The fluctuation-dissipation theorem," Rep. Prog. Phys. **29**, 255 (1966).

[4] T. Herfurth and T. Tchumatchenko, "How linear response shaped models of neural circuits and the quest for alternatives," Curr. Opin. Neurobiol. **46**, 234–240 (2017).

[5] C. E. Leith, "Climate response and fluctuation dissipation," J. Atmos. Sci. **32**, 2022–2026 (1975).

[6] G. R. North, R. E. Bell, and J. W. Hardin, "Fluctuation dissipation in a general circulation model," Clim. Dyn. **8**, 259–264 (1993).

[7] A. S. Gritsun and G. Branstator, "Climate response using a three-dimensional operator based on the fluctuation-dissipation theorem," J. Atmos. Sci. **64**, 2558–2575 (2007).

[8] V. Baladi and D. Smania, "Linear response formula for piecewise expanding unimodal maps," Nonlinearity **21**, 677–711 (2008).

[9] V. Baladi, "Linear response, or else," in *Proceedings of ICM, Seoul 2014* (ICM, 2014), Vol. III, pp. 525–545, arXiv:1408.2937 [math.DS].

[10] D. Ruelle, "A review of linear response theory for general differentiable dynamical systems," Nonlinearity **22**, 855–870 (2009).

[11] D. Ruelle, "Linear response theory for diffeomorphisms with tangencies of stable and unstable manifolds—A contribution to the Gallavotti-Cohen chaotic hypothesis," Nonlinearity **31**, 5683 (2018).

[12] A. Sarracino and A. Vulpiani, "On the fluctuation-dissipation relation in non-equilibrium and non-Hamiltonian systems," Chaos **29**, 083132 (2019).

[13] B. Cessac, "Linear response in neuronal networks: From neurons dynamics to collective response," Chaos **29**, 103105 (2019).

[14] C. Maes and K. Netočný, "Nonequilibrium corrections to gradient flow," Chaos **29**, 073109 (2019).

[15] H. Zhang, X. Li, and J. Harlim, "A parameter estimation method using linear response statistics: Numerical scheme," Chaos **29**, 033101 (2019).

[16] R. V. Abramov, "A theory of average response to large jump perturbations," Chaos **29**, 083128 (2019).

[17] A. J. Majda and D. Qi, "Linear and nonlinear statistical response theories with prototype applications to sensitivity analysis and statistical control of complex turbulent dynamical systems," Chaos **29**, 103131 (2019).

[18] T. Bódai, V. Lucarini, and F. Lunkeit, "Can we use linear response theory to assess geoengineering strategies?" Chaos **30**, 023124 (2020).

[19] S. Galatolo, and J. Sedro, "Quadratic response of random and deterministic dynamical systems," Chaos **30**, 023113 (2020).

[20] A. Castro, "Analytical techniques for linear response formulae of equilibrium states," Chaos **30**, 013134 (2020).

[21] C. L. Wormell and G. A. Gottwald, "Linear response for macroscopic observables in high-dimensional systems," Chaos **29**, 113127 (2019).