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Physical Ergodicity and Exact Response Relations for Low-dimensional Maps

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Abstract: Recently, novel ergodic notions have been introduced in order to find physically relevant formulations and derivations of fluctuation relations. These notions have been subsequently used in the development of a general theory of response, for time continuous deterministic dynamics. The key ingredient of this theory is the Dissipation Function Ω, that in nonequilibrium systems of physical interest can be identified with the energy dissipation rate, and that is used to determine exactly the evolution of ensembles in phase space. This constitutes an advance compared to the standard solution of the (generalized) Liouville Equation, that is based on the physically elusive phase space variation rate. The response theory arising in this framework focuses on observables, rather than on details of the dynamics and of the stationary probability distributions on phase space. In particular, this theory does not rest on metric transitivity, which amounts to standard ergodicity. It rests on the properties of the initial *equilibrium*, in which a system is found before being perturbed away from that state. This theory is exact, not restricted to linear response, and it applies to all dynamical systems. Moreover, it yields necessary and sufficient conditions for relaxation of ensembles (as in usual response theory), as well as for relaxation of single systems. We extend the continuous time theory to time discrete systems, we illustrate our results with simple maps and we compare them with other recent theories.

Key words: dissipation function; coarse graining; probability distributions

I. INTRODUCTION

Ruelle developed a theory for the linear response of smooth uniformly hyperbolic dynamical systems [3], that extends the classical picture based on equilibrium time correlation functions to nonequilibrium steady states. Unlike the case of perturbations of equilibrium systems, the response about nonequilibrium steady states requires more than correlation functions computed with the unperturbed distribution. Indeed, dissipative systems are characterized by invariant distributions that are singular with respect to the Lebesgue measure; hence a perturbation may produce a distribution that is in turn singular with respect to the invariant one. Therefore, in hyperbolic systems, the response involves one contribution due to the expanding (unstable) directions of the dynamics, and another one due to the contracting (stable) directions, which is responsible for relaxation to the unperturbed state.

Being mathematically rigorous, this theory constitutes a testbed for any other theory addressing response. On the other hand, it meets various difficulties when applied to physics Ref. [6], because only a limited number of such systems are uniformly hyperbolic and because the directions of the stable and unstable manifolds cannot be disentangled from each other, except in toy models such as those of Ref. [1], with stationary measure supported and smooth on a 1-dimensional manifold, cf. Eq. (8) below. Thus calculations of the two different contributions to response are usually problematic, and alternative approaches desired. Alternative theories are also required to treat large perturbations, as well as cases in which the system does not relax back to the initial unperturbed state.

The authors of Ref. [6] argued that the response of systems with many degrees of freedom should be determined by the properties of the unperturbed state, as in the case of the Fluctuation Dissipation Theorem, even for perturbations of nonequilibrium steady states (NESS). The observation was based on results on systems with noise which, unlike deterministic dissipative systems, enjoy regular invariant probability distributions [8, 9]. Now, also projecting on lower dimensional spaces the singular distributions of deterministic dissipative dynamics, regular distributions are expected [10], so that small perturbations result in absolutely continuous distributions with respect to the projected invariant ones.

A perspective different from the above has been developed in terms of the *Dissipation Function* Ω, that in cases of interest amounts to the dissipated energy rate [15, 16]. This perspective arose in connection with a kind of ergodic property, *physical ergodicity* [11], that is based on probability distributions that, unlike standard ergodicity, are not necessarily stationary [6, 9, 12, 15, 16]. Developed for continuous time invertible dynamics, this theory is called *physical*, because it focuses on observables, rather than on the details of phase space dynamics. In particlar, it does not rest on stringent assumptions such as metric transitivity or uniform hyperbolicity, which are seldom verified in physics. The main characteristics of the entailing response theory, for an initial distribution f_0, are the following [11, 12]:

- Similarly to Green-Kubo's theory, the response of observable ϕ is given by the time correlation function $\langle \Omega; \phi \circ S^t \rangle_0$ of Ω and ϕ computed in $S^t x$ (phase at time t) averaging with respect to f_0.
- Because it uses the exact evolution of probabilities determined by Ω, this response theory is exact and applies to all dynamical systems.[1] Moreover, unlike Green-Kubo's and most response theories, it is not restricted to small perturbations.
- The sufficiently fast decay of that correlation function is a sufficient and, more importantly, a **necessary** condition,[2] called Ωt-mixing, for the relaxation of ensembles to a steady state.[3]
- Ωt-mixing differs from standard mixing because it is computed with respect to one non-invariant (*i.e. transient*) distribution, instead of an invariant distribution. Unlike mixing, that expresses the loss of microscopic correlations within a given macrostate, Ωt-mixing expresses the loss of correlations among macrostates, which is why it describes relaxation processes.
- In general, response theories do not address the evolution of a single system: they express the response in terms of ensemble averages. Close to equilibrium for macroscopic objects, it can be safely assumed that the behavior of the average over an ensemble of systems is the same as the behavior of a generic single member of the ensemble, but away from equilibrium or for small systems, single ensemble members can have different behaviors (cf. a single pollen grain in the Brownian motion). The condition called t-mixing in this paper, guarantees that single systems behave like their ensemble, apart from exceptions that only cover a vanishing phase space volume. For dissipative systems this is not the ergodic condition, since ergodicity for dissipative systems only concerns a set of zero phase space volume.
- One advantage of using Ω as the propagator of the evoultion of phase space probabilities, as opposed to direct integration of the (generalized) Liouville equation, in terms of the phase space variation rate Λ, is that unlike Λ, Ω is a physically measurable quantity.[4]

Here, we extend this exact theory of response to discrete-time systems, including non-invertible maps, and we compare it with other nonequilibrium response theories. We show that our theory yields the correct results in cases in which Ruelle's theory applies, while it still provides a viable tool (for both analytical and numerical calculations) in cases in which Ruelle's theory does not apply. Moreover, we illustrate the difference between single system and ensemble behaviors, for two Ωt-mixing maps.

Section II illustrates Ruelle's linear response about nonequilibrium steady states by means of simple maps. Section III presents the corresponding alternative approach, based on coarse grained distributions, developed in Ref. [6]. Section IV is devoted to the definition of Ω, to its use in the derivation of the steady state fluctuation relations via the decay of transient states correlations. Section V introduces the t-mixing and Ωt-mixing conditions, suggested by the decay of transient states correlations of Section IV. Moreover, in Section V, these notions are extended to discrete time dynamics and they are used for the corresponding response of various examples. Section VI contains concluding remarks.

[1] Such generality implies that the response may have different physical interpretations, depending on the system under consideration. For instance, in certain cases response formulae express only the average behavior of one ensemble of systems, while in other cases they express the behavior of a single system.

[2] Sufficient conditions tend to be too strong for physics purposes, and to highlight aspects alien to the systems of interest. Being *"necessarily"* verified when certain phenomena (*e.g.* relaxation) occur, necessary conditions highlight relevant mechanisms.

[3] At the moment the definitions concerning the notion of t-mixing are not fully settled. The first instance in which the notion appears is Ref. [16], but no name was given to it. Further, what we call t-mixing in this paper is sometimes called weak-t-mixing. The book [17] is likely to set the standard terminology.

[4] This observation is limited to the issue of computing response explicitly from the evolution of probability densities. The conclusion that *"the close relationship linking phase volume to thermodynamics is to be celebrated rather than avoided"* in Ref. [13] is of course valid. Much of nonequilibrium phenomena has been understood thanks to the relation between the average phase space contraction rate and entropy production.

II. RUELLE'S LINEAR RESPONSE THEORY

In this section we summarize Ruelle's theory, from the perspecitve of Ref. [1], in which examples with clearly identified stable and unstable manifolds have been explicitly worked out. Along the unstable manifold one can apply the standard Green-Kubo linear response theory, that yields the linear response to a perturbation as a time correlation function of the system at equilibrium. This is due to the fact that the probability measure is smooth along the unstable direction, and an impulse along that direction results in an equally smooth distribution. We call *unstable response function* the corresponding contribution to the response formula. This must be complemented by the contribution due to the stable direction, that we call *stable response function*, and that is not expressed by a correlation function. One then obtains susceptibilities showing two different kinds of resonances, named *unstable* and *stable* resonances. For concreteness consider a map:

$$\mathbf{x}_{t+1} = \mathbf{F}(\mathbf{x}_t) \tag{1}$$

with $t \in \mathbb{Z}$, $\mathbf{x} \in M$, where M is the phase space and $\mathbf{F}$ is smooth but not necessarily invertible. Let this dynamics be chaotic, mixing and associated with an ergodic Sinai-Ruelle-Bowen (SRB) measure, so that the time average of the observable $A(\mathbf{x})$

$$\overline{A} = \lim_{T\to\infty} \frac{1}{T} \sum_{t=0}^{T-1} A(\mathbf{F}^t(\mathbf{x})) \tag{2}$$

equals the ensemble average:

$$\langle A \rangle = \int \rho_F(d\mathbf{x}) A(\mathbf{x}) = \lim_{t\to\infty} \int d\mathbf{x} A(\mathbf{F}^t(\mathbf{x})) \tag{3}$$

for almost all initial conditions $\mathbf{x}$ selected with respect to the Lesbegue (volume) measure $d\mathbf{x}$. A time dependent perturbation is then introduced, producing the new dynamics

$$\tilde{\mathbf{x}}_{t+1} = \tilde{\mathbf{F}}_t(\tilde{\mathbf{x}}_t) + \xi_{t+1}(\tilde{\mathbf{x}}_t), \tag{4}$$

where $\xi_{t+1}(\mathbf{x})$ defines the perturbation. The tilde, meant to distinguish the perturbed from the unperturbed dynamics, will be omitted when there is no risk of confusion. One would then like to compute the mean values $\langle A \rangle_t$ at all times of the observables for the perturbed dynamics. This is not trivial, in general, also because the asymptotic state could differ from the unperturbed state, and be unknown.

Among the possible perturbations of the system, a special role is played by the impulse perturbation, because the linear response to generic perturbations can be expressed as a linear combination of impulse responses at different times. The following formula holds for the impulse response:

$$\begin{aligned} \chi_{A\xi}(t-\tau) &= \langle A \rangle_t - \langle A \rangle = \\ &= \int \rho_F(d\mathbf{x})\, \nabla(A \circ \mathbf{F}^{t-\tau})(\mathbf{F}(\mathbf{x}))\cdot\xi(\mathbf{x}). \end{aligned} \tag{5}$$

Introducing the time-dependent perturbation as a sum of impulses, $\xi_t(\mathbf{x}) = \sum_{\tau=-\infty}^{t} \xi_\tau(\mathbf{x})$, the linear response is then given by:

$$\langle \delta A \rangle_t = \sum_{\tau=-\infty}^{t} \chi_{A\xi}(t-\tau). \tag{6}$$

Ruelle [2] has proven that the series converges for uniformly hyperbolic systems. In particular, the unstable response converges because of exponential mixing and is given by a correlation function. At the same time, the stable part converges due to phase space contraction. A straightforward application of equations (5) and (6) is represented by the linear response to a periodic perturbation of the form $\xi_t(\mathbf{x}) = \xi(\mathbf{x})e^{-i\omega t}$. In this case, the linear response of observable A reads:

$$\langle \delta A \rangle_t = \tilde{\chi}_{A\xi}(\omega) e^{-i\omega t}\,, \quad \text{with } \tilde{\chi}_{A\xi}(\omega) = \sum_{t=-\infty}^{\infty} \chi_{A\xi}(t) e^{i\omega t}, \tag{7}$$

where the complex amplitude $\tilde{\chi}_{A\xi}$ is called *susceptibility*, and $\chi_{A\xi}(t) = 0$ for $t < 0$. The authors of Ref. [1] applied this theory to the following chaotic rotator in the plane,

$$\begin{aligned} \theta_{t+1} &= g(\theta_t, r_t) + \epsilon_\theta \xi_\theta(t+1, \theta_t, r_t)\,, \\ r_{t+1} &= R(r_t) + \epsilon_r \xi_r(t+1, \theta_t, r_t) \end{aligned} \tag{8}$$

with $g(\theta) = 2\theta \mod 1$, $R(r) = 1 + e^{-\mu}(r-1)$ and $\mu > 0$. Here, the stable and the unstable directions are clearly separated, and we have a chaotic (non-fractal) attractor. Because of the mod operation, the map is not invertible: each θ_t at time t has two pre-images at time $t-1$.

In this two dimensional case, one has an impulse response matrix, whose entries are given by

$$\begin{aligned} \chi_{ij}(t) &= \int \rho_F(dxdy) \nabla F_i^t(F(x,y))\cdot(\xi_j(x,y)\mathbf{e}_j) = \\ &= \int \rho_F(dxdy) \nabla F_i^t(x,y)\cdot(X_j(x,y)\mathbf{e}_j). \end{aligned} \tag{9}$$

For invertible dynamics, $X_j = \xi_j \circ \mathbf{F}^{-1}$. In our non-invertible case, X_j is an average over all pre-images. Moreover, the non-diagonal terms of the response matrix vanish because the unperturbed dynamics of the two variables are decoupled. For the diagonal elements, we have:[5]

$$\begin{aligned} \chi_{\theta\theta}(t) &= \int \rho_F(rdrd\theta) \partial_\theta g^t(\theta) X_\theta(\theta, r) \\ &\doteq -\langle \theta_t; \partial_\theta X_\theta(\theta_0, 1) \rangle, \end{aligned} \tag{10}$$

[5] Introducing the *time correlation function* $\langle A(\mathbf{x}_t); B(\mathbf{x}_0) \rangle \doteq \int \rho_F(d\mathbf{x}) A(\mathbf{F}^t(\mathbf{x})) B(\mathbf{x}) - \langle A \rangle \langle B \rangle$ of A and B.

$$\chi_{rr}(t) = \int \rho_F(rdrd\theta)\partial_r R^t(r) X_r(\theta, r) = e^{-\mu t}\langle X_r(\theta, 1)\rangle. \tag{11}$$

As a concrete example with non-vanishing $\chi_{\theta\theta}$, let us take the following θ-dependent perturbation

$$\begin{aligned} &X_\theta(\theta) = 6\theta(1-\theta)\ ,\ \text{that yields} \\ &\chi_{\theta\theta}(t) = 12\langle\theta_t;\theta_0\rangle = 2^{-t}\ \text{ for }\ t > 0. \end{aligned} \tag{12}$$

The corresponding susceptibility:

$$\tilde{\chi}_{\theta\theta}(\omega) = \frac{1}{1 - e^{i(\omega + i\log 2)}} \tag{13}$$

has a complex pole in $\omega = -i\log 2$ on the imaginary axis, which is known as a Ruelle-Policott resonance [4, 5]. In turn, the susceptibility of Eq. (11) reads:

$$\tilde{\chi}_{rr}(\omega) = \frac{C}{1 - e^{i(\omega + i\mu)}}, \tag{14}$$

which has a pole in $\omega = -i\mu$ that does not depend on the ones of the correlation function. This simple example effectively illustrates how the response of the system is affected by the two types of perturbation: the perturbation parallel to the unstable direction and the one parallel to the stable direction.

III. COARSE GRAINING

In Ruelle's theory, the unstable response is related to the dynamics on the attractor, while the stable response may not. The reason is that the stationary probability distributions of dissipative dynamics are singular, and perturbations along the stable direction may lead to microscopic phases of zero probability in the unperturbed state. Then, the information carried by the unperturbed stationary probability distribution is irrelevant, and the stable contribution to linear response must be separately computed.

Reference [6] argues, however, that this difficulty does not seriously affect systems of many interacting particles. Indeed, in those cases one usually considers much lower dimensional projections of the phase space than the phase space itself, and the projections of the corresponding probability distributions are expected to be smooth, rather than singular [7, 10]. The fact is that one is usually interested on several physically relevant observables, not on the fine details of the phase space distributions.

Reference [6] then proposes an alternative approach to linear response about nonequilibrium steady states. For a dissipative dynamical system with a d-dimensional phase space, let the impulsive perturbation $\delta\Gamma$ consist of vanishing components, except the i-th component denoted $\delta\Gamma_i$. The probability distribution μ is then shifted by $\delta\Gamma$, producing a non-invariant distribution, μ_0 say, defined by $\mu_0(E) = \mu(E - \delta\Gamma)$ for every measurable set E.[6] It is further assumed that the time evolution of μ_0, μ_t, relaxes back to μ in the course of time. Taking the observable $\phi(\Gamma) = \Gamma_i$, one can write:

$$\langle\Gamma_i\rangle_t - \langle\Gamma_i\rangle_0 = \int \Gamma_i\ \mathrm{d}\mu_t(\Gamma) - \int \Gamma_i\ \mathrm{d}\mu(\Gamma). \tag{15}$$

To compute this response, the singular μ and μ_t are approximated by coarse graining the phase space $\mathcal{M}$ with a finite partition made of d-dimensional hypercubes $\Lambda_k(\epsilon)$ of side ϵ and centers Γ_k. Introducing the probabilities $P_k(\epsilon)$ and $P_{t,k}(\epsilon;\delta\Gamma)$ of the hypercubes $\Lambda_k(\epsilon)$:

$$P_k(\epsilon) = \int_{\Lambda_k(\epsilon)} \mathrm{d}\mu(\Gamma)\ ,\quad P_{t,k}(\epsilon;\delta\Gamma) = \int_{\Lambda_k(\epsilon)} \mathrm{d}\mu_t(\Gamma)\ , \tag{16}$$

the invariant distribution is approximated by the coarse grained density $\rho(\Gamma;\epsilon)$, defined by:

$$\begin{aligned} &\rho(\Gamma;\epsilon) = \sum_k \rho_k(\Gamma;\epsilon)\ ,\quad \text{with} \\ &\rho_k(\Gamma;\epsilon) = \begin{cases} P_k(\epsilon)/\epsilon^d & \text{if } x \in \Lambda_k(\epsilon) \\ 0 & \text{else.} \end{cases} \end{aligned} \tag{17}$$

If Z_i is the number of one-dimensional bins of form $\left[\Gamma_i^{(q)} - \epsilon/2, \Gamma_i^{(q)} + \epsilon/2\right)$, $q \in \{1, 2, ..., Z_i\}$, in the i-th direction, marginalizing the approximate distribution yields the quantities:

$$p_i^{(q)}(\epsilon) = \int_{\Gamma_i^{(q)} - \frac{\epsilon}{2}}^{\Gamma_i^{(q)} + \frac{\epsilon}{2}} \left\{ \int \rho(\Gamma;\epsilon) \prod_{j\neq i} \mathrm{d}\Gamma_j \right\} \mathrm{d}\Gamma_i, \tag{18}$$

each of which is the invariant probability that the coordinate Γ_i of Γ lie in the q-th bin. Similarly, one gets the marginal of the evolving approximate probability:

$$p_{i,t}^{(q)}(\epsilon) = \int_{\Gamma_i^{(q)} - \frac{\epsilon}{2}}^{\Gamma_i^{(q)} + \frac{\epsilon}{2}} \left\{ \int \rho_t(\Gamma;\epsilon) \prod_{j\neq i} \mathrm{d}\Gamma_j \right\} \mathrm{d}\Gamma_i. \tag{19}$$

Dividing by ϵ, one obtains the coarse grained marginal probability densities $\rho_i^{(q)}(\epsilon)$ and $\rho_{t,i}^{(q)}(\epsilon)$, as well as the ϵ-approximate response function:

$$\begin{aligned} &B_i^{(q)}(\Gamma_i, \delta\Gamma, t, \epsilon) = \frac{1}{\epsilon}\left[p_{t,i}^{(q)}(\epsilon) - p_i^{(q)}(\epsilon)\right] = \\ &= \rho_{t,i}^{(q)}(\epsilon) - \rho_i^{(q)}(\epsilon). \end{aligned} \tag{20}$$

The right hand side of Eq. (20) tends to a regular function of Γ_i under the $Z_i \to \infty$, $\epsilon \to 0$ limits [6]. Consequently, $B_i^{(q)}(\Gamma_i, \delta\Gamma, t, \epsilon)$ yields an expression analogous to that of standard response theory, that depends solely on the unperturbed state. There are of course exceptions, but for most macroscopic systems, this is the expected result. The idea is that the projection procedure makes unnecessary the explicit calculation of the stable response [1]. Therefore, the linear

[6] The set $E - \delta\Gamma$ is defined by $\{\Gamma \in \mathcal{M} : \Gamma + \delta\Gamma \in E\}$.

response may be typically computed only in terms of the unperturbed dynamics, as in the classical theory.

The peculiarity of dynamics like Eq. (8), in relation to response theory, appears also within this coarse graining approach. Coarse graining is indeed commonly used to overcome difficulties related to the singularity of phase space probability distributions [18]. Although its physical justification constitutes a delicate issue, especially in nonequilibrium situations [19-21], the coarse graining procedure succeeds, formally at least, because the usual invariant distributions spread over most of the phase space [22], and the stable and the unstable directions (when they exist) are finely intertwined with each other.

Unlike such situations, the attractor of Eq. (8) is concentrated on a vanishing part of the phase space, because the two coordinates trivially identify the unstable and the stable directions. After coarse graining in the r direction with bins of form $[r^{(q)} - \frac{\epsilon}{2}, r^{(q)} + \frac{\epsilon}{2}]$, the singular distribution $d\mu(r) = \delta(r-1)dr$ is approximated by a density that takes value $\rho_{r,\epsilon} = \frac{1}{\epsilon}$ on the finite volume $[1 - \frac{\epsilon}{2}, 1 + \frac{\epsilon}{2}]$ and vanishes elsewhere. The impulsive perturbation of this density therefore produces $\mu_{0,\epsilon}(r) = \mu(r - \delta r)$ that is positive in one or two bins, and vanishes elsewhere. Therefore, the problem of falling in regions of vanishing unperturbed probability persists in this example, despite the coarse graining.

IV. FROM FLUCTUATION RELATIONS TO THE DISSIPATION FUNCTION

The above two theories represent popular approaches to nonequilibrium systems and, in particular, to linear response about nonequilibrium steady states: **a)** the mathematically rigorous approach that yields sufficient conditions for certain results to hold, hence it rests on dynamical assumptions that are hard to verify and may be alien to the physics of interest; **b)** the coarse graining approach, that values the stochasticity typical of observations at mesoscopic scales, and that must be properly controlled to avoid subjective features not present in the physical phenomena. Considering that, in any case, linear response is insufficient in many nonequilibrium situations, more complete theories are welcome. Below we focus on one such theory, that has emerged within the study of fluctuation relations (FR).

IV. 1. Fluctuation Relations

In 1993, the paper [14] addressed the question of the fluctuations of the entropy production rate in a pioneering attempt towards a unified theory of nonequilibrium phenomena. The FR derived in [14] was at the time one of the very few exact results for systems almost arbitrarily far from equilibrium, and close to equilibrium it reduces to the Green-Kubo and Onsager relations. This FR reads:

$$\frac{\mathrm{Prob}_\tau(\sigma \approx A)}{\mathrm{Prob}_\tau(\sigma \approx -A)} = e^{\tau A}, \tag{21}$$

where A and $-A$ are averages over a long time τ of the entropy production rate σ, and $\mathrm{Prob}_\tau(\sigma \approx \pm A)$ is the steady state probability of observing values close to $\pm A$. Equation (21) is a *large deviation* relation, since for large τ any $A \neq \langle\sigma\rangle$ lies many standard deviations away from the mean. The FR is parameter-free and, being dynamical in nature, it applies almost arbitrarily far from equilibrium and to large as well as to small systems.

Gallavotti and Cohen framed the FR within the theory of Anosov systems [24, 25]. As the Anosov property practically means a high degree of randomness, analogous results have been obtained first for finite state space Markov chains and later for many other stochastic processes [9]. However, the Anosov framework meets various difficulties [9, 23], hence an alternative approach has been developed [16].

IV. 2. FR for the dissipation function

Investigating the mechanisms under which the FR holds for the energy dissipation of many nonequilibrium systems, a kind of ergodic notion called *t-mixing* has been introduced, and one general response formula has been derived. This study originates with Refs. [26, 27] by Evans and Searles, who proposed the first transient FR for the *Dissipation Function* Ω. This FR seems similar to Eq. (21) but is indeed of a different nature; it is obtained under virtually no hypothesis except for *time reversibility*, and it is called transient because it concerns non-invariant ensembles, instead of the steady state.

To summarize its derivation (for further details, see the review article [28]) let $\mathcal{M}$ be the phase space, and $I : \mathcal{M} \to \mathcal{M}$ be the time reversal operation. Let $S^\tau : \mathcal{M} \to \mathcal{M}$ be a reversible evolution, *i.e.* $IS^\tau = S^{-\tau} I$, solution of $\dot{\Gamma} = F(\Gamma)$. Denote time averages by:

$$\overline{\mathcal{O}}_{t,t+\tau}(\Gamma) \doteq \frac{1}{\tau}\mathcal{O}_{t_0,t_0+\tau}(\Gamma) \doteq \frac{1}{\tau}\int_{t_0}^{t_0+\tau} \mathcal{O}(S^s\Gamma)ds \,. \tag{22}$$

For a probability measure $d\mu_0(\Gamma) = f_0(\Gamma)d\Gamma$ on $\mathcal{M}$, with even density f_0 under time reversal, *i.e.* $f_0(I\Gamma) = f_0(\Gamma)$, let us define the

Dissipation function:

$$\begin{aligned} \Omega(\Gamma) &= -\frac{d}{d\Gamma}\log f_0\Big|_\Gamma \cdot \dot{\Gamma} - \Lambda(\Gamma) \,, \quad \text{so that} \\ \overline{\Omega}_{t,t+\tau}(\Gamma) &= \frac{1}{\tau}\left[\log\frac{f_0(S^t\Gamma)}{f_0(S^{t+\tau}\Gamma)} - \Lambda_{t,t+\tau}\right] \end{aligned} \tag{23}$$

Here Λ is the phase space expansion rate defined as $\Lambda(\Gamma) = \log J(\Gamma)$, where J is the Jacobian determinant of S. It turns out that Ω can be identified with the *entropy production rate* σ, or more generally with the dissipated power, if f_0 is an appropriate equilibrium ensemble [16, 26, 27]. The existence of the logarithmic term in (23) is called *ergodic consistency*, a condition met if $f_0 > 0$ in all regions visited by all trajectories $S^t\Gamma$.

Take $\delta > 0$, the set $A_\delta^\pm = (\pm A - \delta, \pm A + \delta)$, and let $E(\mathcal{O} \in (a,b))$ be the set of points Γ such that $\mathcal{O}(\Gamma) \in (a,b)$. Then, we have $E(\overline{\Omega}_{0,\tau} \in A_\delta^-) = IS^\tau E(\overline{\Omega}_{0,\tau} \in A_\delta^+)$ and:

$$\frac{\mu_0(E(\overline{\Omega}_{0,\tau} \in A_\delta^-))}{\mu_0(E(\overline{\Omega}_{0,\tau} \in A_\delta^+))} \doteq \frac{\int_{E(\overline{\Omega}_{0,\tau} \in A_\delta^+)} f_0(S^\tau X) e^{-\Lambda_{0,\tau}(X)} dX}{\int_{E(\overline{\Omega}_{0,\tau} \in A_\delta^+)} f_0(\Gamma) d\Gamma}$$
$$= \frac{\int_{E(\overline{\Omega}_{0,\tau} \in A_\delta^+)} e^{-\Omega_{0,\tau}(X)} f_0(X) dX}{\int_{E(\overline{\Omega}_{0,\tau} \in A_\delta^+)} f_0(\Gamma) d\Gamma} \doteq \left\langle e^{-\Omega_{0,\tau}} \right\rangle_{\overline{\Omega}_{0,\tau} \in A_\delta^+}, \tag{24}$$

where by $\langle \cdot \rangle_{\overline{\Omega}_{0,\tau} \in A_\delta^+}$ we mean the average computed with respect to μ_0 under the condition that $\overline{\Omega}_{0,\tau} \in A_\delta^+$. The transient Ω-FR immediately follows:

$$\frac{\mu_0(E(\overline{\Omega}_{0,\tau} \in A_\delta^+))}{\mu_0(E(\overline{\Omega}_{0,\tau} \in A_\delta^-))} = e^{[A + \epsilon(\delta, A, \tau)]\tau}, \tag{25}$$

where $|\epsilon(\delta, A, \tau)|$ is a correction term not larger than δ.

The transient Ω-FR refers to the non-invariant distribution μ_0, hence its similarity with the steady state FR (21) is only apparent. Rather than expressing a statistical property of fluctuations of a given system in a steady state, Eq. (25) expresses a property of the equilibrium ensemble f_0, using the (nonequilibrium) dynamics S. Therefore, the transient Ω-FR closes the circle with the Fluctuation Dissipation Relation, that obtains non equilibrium properties from equilibrium experiments.

The steady state Ω-FR requires further hypotheses. Consider $\hat{t} = t + \tau + t$ and the coordinate transformation $\Gamma = IS^{\hat{t}} W$ in $\mathcal{M}$. Then, some algebra yields:

$$\frac{\mu_0(E(\overline{\Omega}_{t,t+\tau} \in A_\delta^-))}{\mu_0(E(\overline{\Omega}_{t,t+\tau} \in A_\delta^+))} = \left\langle \exp\left(-\Omega_{0,\hat{t}}\right) \right\rangle_{\overline{\Omega}_{t,t+\tau} \in A_\delta^+} =$$
$$= e^{[A + \epsilon(\delta, t, A, \tau)]\tau} \left\langle e^{-\Omega_{0,t} - \Omega_{t+\tau, 2t+\tau}} \right\rangle_{\overline{\Omega}_{t,t+\tau} \in A_\delta^+}, \tag{26}$$

where $|\epsilon(\delta, t, A, \tau)| \le \delta$ and the second line follows from the first because $\Omega_{0,\hat{t}} = \Omega_{0,t} + \Omega_{t,t+\tau} + \Omega_{t+\tau,\hat{t}}$ with the central contribution approximately equal to A. Recall that $\mu_0(E) = \mu_t(S^t E)$, where μ_t is the evolved probability distribution, with density f_t. Then, taking the logarithm, dividing by τ, and recalling that $E(\overline{\Omega}_{0,\tau}) = S^t E(\overline{\Omega}_{t,t+\tau})$ leads to:

$$\frac{1}{\tau} \log \frac{\mu_t(E(\overline{\Omega}_{0,\tau} \in A_\delta^+))}{\mu_t(E(\overline{\Omega}_{0,\tau} \in A_\delta^-))} = A + \epsilon(\delta, t, A, \tau)$$
$$-\frac{1}{\tau} \log \left\langle e^{-\Omega_{0,t} - \Omega_{t+\tau, 2t+\tau}} \right\rangle_{\overline{\Omega}_{t,t+\tau} \in A_\delta^+} \tag{27}$$
$$\doteq A + \epsilon(\delta, t, A, \tau) + M(A, \delta, t, \tau).$$

If μ_t tends to a steady state μ_∞ when $t \to \infty$, the exact relation (27) changes from a statement on the ensemble f_t, to a statement concerning also the statistics of a single typical trajectory. Moreover, provided $M(A, \delta, t, \tau)$ vanishes with growing τ, one has the steady state FR for Ω:

$$\lim_{\tau \to \infty} \frac{1}{\tau} \log \frac{\mu_\infty(E(\overline{\Omega}_{0,\tau} \in A_\delta^+))}{\mu_\infty(E(\overline{\Omega}_{0,\tau} \in A_\delta^-))} = A + \eta, \text{ with } \eta \in (-\epsilon, \epsilon) \tag{28}$$

The problem is that $M(A, \delta, t, \tau)$ could instead diverge with growing t, before the $\tau \to \infty$ is taken. This happens if one of the probabilities on the left hand side of Eq. (27) vanishes, *i.e.* if A or $-A$ are not observable in the steady state, in which case there is no need for the FR. Therefore, let us assume that A and $-A$ are observable, and note that Eqs.(23) imply

$$f_s(\Gamma) = f_0\left(S^{-s}\Gamma\right) e^{-\Lambda_{-s,0}(\Gamma)} = f_0(\Gamma) e^{\Omega_{-s,0}(\Gamma)} \tag{29}$$

from which one immediately gets $\left\langle e^{-\Omega_{0,s}} \right\rangle_0 = 1$ for every $s \in I\!R$. Moreover, if the Ω-autocorrelation with respect to f_0 decays instantaneously in time, so that:

$$1 = \left\langle e^{-\Omega_{0,s} - \Omega_{s,t}} \right\rangle_0 = \left\langle e^{-\Omega_{0,s}} \right\rangle_0 \left\langle e^{-\Omega_{s,t}} \right\rangle_0, \tag{30}$$

one obtains

$$\left\langle e^{-\Omega_{s,t}} \right\rangle_0 = 1, \quad \text{for all } s \text{ and } t \tag{31}$$

and the conditional average of eq.(27) does not depend on the condition $\overline{\Omega}_{t,t+\tau} \in A_\delta^+$:

$$\left\langle e^{-\Omega_{0,t}} \cdot e^{-\Omega_{t+\tau, 2t+\tau}} \right\rangle_{\overline{\Omega}_{t,t+\tau} \in A_\delta^+} =$$
$$= \left\langle e^{-\Omega_{0,t}} \cdot e^{-\Omega_{t+\tau, 2t+\tau}} \right\rangle_0 = 1. \tag{32}$$

Then, the logarithmic term in Eq. (27) identically vanishes for all t, τ, and the steady state Ω-FR is verified at all $\tau > 0$. Although such an idealized situation may not be realized, molecular dynamics indicates that for τ larger than a characteristic time τ_M, one may write [16]:

$$\left\langle e^{-\Omega_{0,t}} \cdot e^{-\Omega_{t+\tau, 2t+\tau}} \right\rangle_0 \approx$$
$$\approx \left\langle e^{-\Omega_{0,t}} \right\rangle_0 \left\langle e^{-\Omega_{t+\tau, 2t+\tau}} \right\rangle_0 = O(1), \tag{33}$$

where $\left\langle e^{-\Omega_{s,t}} \right\rangle_0 = \left\langle e^{-\Omega_{0,t-s}} \right\rangle_s$. If this scenario is realized, $M(A, \delta, \tau)$ vanishes as $1/\tau$ with τ.

Equations (30) and (33) represent a kind of mixing property, which refers to the non-invariant distribution μ_0, unlike the standard notion of mixing that concerns invariant distributions.

IV. 3. Dissipation function, t-mixing and response

Equations (30) and (33) are one instance of the following property for two observables ϕ and ψ:

$$\lim_{t \to \infty} \left[\left\langle \psi \left(\phi \circ S^t\right) \right\rangle_0 - \langle \psi \rangle_0 \langle \phi \rangle_t\right] = 0 \tag{34}$$

where $\phi \circ S^t \Gamma = \phi(S^t \Gamma)$. This condition is called *t-mixing*.

For $\psi = \Omega$ one has $\langle \Omega \rangle_0 = 0$ because Ω is odd and f_0 is even under time reversal, hence Eq. (34) turns to

$$\lim_{t \to \infty} \left\langle \Omega \left(\phi \circ S^t\right) \right\rangle_0 = 0 \tag{35}$$

If the decay of this correlation is faster than $1/t$, the condition called Ωt-*mixing* holds, *i.e.* the following integral

$$\int_0^\infty \left\langle \Omega\left(\phi \circ S^t\right)\right\rangle_0 \, \mathrm{d}t \tag{36}$$

converges (it is a real number). This is important because Eq. (29) leads to the identity [29]:

$$\langle\phi\rangle_t = \langle\phi\rangle_0 + \int_0^t \mathrm{d}s \, \left\langle \Omega\left(\phi \circ S^s\right)\right\rangle_0 \tag{37}$$

that holds for all positive times t. Hence Ωt-mixing implies the following response formula:

$$\langle\phi\rangle_t \stackrel{t\to\infty}{\longrightarrow} \langle\phi\rangle_0 + \int_0^\infty \mathrm{d}s \, \left\langle \Omega\left(\phi \circ S^s\right)\right\rangle_0 \in I\!R. \tag{38}$$

Standard mixing concerns steady states and correlations decay of microscopic phases within a steady state; t-mixing concerns instead evolving distributions, hence correlations decay of macrostates [12, 29].

V. DISSIPATION FUNCTION AND RESPONSE FOR MAPS

To investigate maps as in Sections 2 and 3, we extend the above continuous time response theory to discrete time dynamics, integrating it over a unitary time interval. For instance, $\dot{x} = \Lambda x$ yields

$$S^t x_0 = e^{\Lambda t} x_0 \,, \quad \text{hence} \quad x_1 = S^1 x_0 = e^{\Lambda} x_0. \tag{39}$$

For the evolution of probability densities, observe that the conservation of probability yields:

$$\int_E f_0(x)dx = \int_{S^1 E} f_1(y)dy, \tag{40}$$

where E is a subset of $\mathcal{M}$. Then, the change of variables $y(x) = S^1 x = e^\Lambda x$ leads to

$$f_0(x) = f_1(S^1 x)e^\Lambda. \tag{41}$$

Using Eqs.(23) we now replace the continuous time with the **discrete time dissipation function**:

$$\begin{aligned}\Omega(x) \doteq \Omega_{0,1}(x) = \log\frac{f_0(x)}{f_0(S^1 x)} - \int_0^1 \Lambda(S^s x)ds = \\ = \log\frac{f_0(x)}{e^\Lambda}\frac{1}{f_0(S^1 x)} = \log\frac{f_1(S^1 x)}{f_0(S^1 x)},\end{aligned} \tag{42}$$

where

$$\begin{aligned} f_1(S^1 x) = f_0(S^1 x)e^{\Omega_{0,1}(x)} \quad \text{and} \\ f_1(x) = f_0(S^{-1}x)e^{\Omega_{0,1}(S^{-1}x)}.\end{aligned} \tag{43}$$

Iterating t times Eq. (43), the **discrete time response formula** for a generic observable ϕ takes the form:

$$\begin{aligned}\langle\phi\rangle_t - \langle\phi\rangle_0 &= \int_{\mathcal{M}} \phi(x)\Big[f_t(x) - f_0(x)\Big]dx \\ &= \int_{\mathcal{M}} \phi(x)\Big[e^{\Omega_{0,t}(S^{-t}x)} - 1\Big] f_0(x)dx \\ &= \Big\langle \phi \, e^{\Omega_{0,t}\circ S^{-t}} \Big\rangle_0 - \langle\phi\rangle_0,\end{aligned} \tag{44}$$

where

$$\Omega_{0,t}\left(S^{-t}x\right) = \sum_{k=0}^{t-1} \Omega\left(S^{k-t}x\right) = \sum_{k=1}^{t} \Omega\left(S^{-k}x\right). \tag{45}$$

If S^{-1} is multivalued, as for Eqs.(8), all pre-images of the phase space points must be considered.

Equation (44) replaces Eq. (37) for $t \in I\!N$ (compare also with Eq. (16) of Ref. [30]). Like Eq. (37), it is an exact and completely general identity, that is merely based on probability conservation; the dynamics does not need to satisfy any special property for Eq. (44) to hold. Like Eq. (37), Eq. (44) rests on the transient time correlation function of Ω and ϕ. Furthermore, f_0 must be positive on all points in the accessible phase space, as in the case of equilibrium distributions.[7] Condition (36) is now replaced by the **discrete time Ωt-mixing condition**:

$$\lim_{t\to\infty} \langle \phi \, e^{\Omega_{0,t}\circ S^{-t}} \rangle_0 \in I\!R \tag{46}$$

Analogously to Eq. (36), Eq. (46) is **necessary and sufficient** for relaxation of the initial ensemble to an invariant ensemble, because Eq. (44) is an exact identity.

V. 1. Response for purely expanding dynamics

Consider the first of Eqs.(8), and endow its phase space $\mathcal{M} = [0, 1)$ with the invariant distribution:

$$d\mu_0(\theta) = f_0(\theta)d\theta = d\theta. \tag{47}$$

Equation (45) implies the following expression for the dissipation function:

$$\Omega_{0,t} = \log\frac{f_0(\theta)}{f_0(S^t\theta)} - \sum_{k=1}^{t} \log 2 \; ds = -t\log 2. \tag{48}$$

In order to apply Eq. (44), we note that a point $\theta \in \mathcal{M}$ has, at a given time t, 2^t pre-images, so that

$$\langle\theta\rangle_t = \int_0^1 d\theta \; \theta \; e^{\Omega_{0,t}\circ S^{-t}} = \int_0^1 d\theta \; \theta \; \sum_{k=1}^{2^t} e^{-t\log 2} = \frac{1}{2}. \tag{49}$$

[7] In general, this condition can be easily realized by restricting the analysis to the ostensible phase space.

This value is constant in time, because the uniform probability measure is invariant. To investigate how our formalism relates to the one of Sec.II., we perturb this distribution with the impulse $6\epsilon\theta(1-\theta)$ [1]. Then, θ_1 can be expressed as a function of θ_0, as follows

$$6\epsilon\theta_1^2 + (1-6\epsilon)\theta_1 - 2\theta_0 \mod 1 = 0 \tag{50}$$

and we have two cases.

- $\theta_0 \in [0, \frac{1}{2})$, which requires $6\epsilon\theta_1^2+(1-6\epsilon)\theta_1-2\theta_0 = 0$ and to first order in ϵ yields

$$\begin{aligned} &\theta_1 = 2\theta_0 + \xi_1(\theta_0)\epsilon + O(\epsilon^2)\ , \quad \text{with} \\ &\xi_1(\theta) = 12\theta - 24\theta^2. \end{aligned} \tag{51}$$

- $\theta_0 \in [\frac{1}{2}, 1)$, which requires $6\epsilon\theta_1^2 + (1-6\epsilon)\theta_1 - 2\theta_0 + 1 = 0$ and to first order in ϵ yields:

$$\begin{aligned} &\theta_1 = 2\theta_0 - 1 + \xi_2(\theta_0)\epsilon + O(\epsilon^2), \\ &\xi_2(\theta) = -24\theta^2 + 36\theta - 12. \end{aligned} \tag{52}$$

The perturbed distribution after one time step can be computed as follows.

- Consider $\theta \in [0, \frac{1}{2}]$ and recall that $f_0(\theta) = 1$. Then, take the mapping $\theta \to 2\theta + \epsilon\xi_1(\theta)$ from Eq. (51), which is invertible in $[0, \frac{1}{2})$ if $\epsilon < \frac{1}{6}$. Consequently,

$$\begin{aligned} &f_0(\theta) = f_1(S^1\theta)\frac{d}{d\theta}S^1\theta \quad \text{and} \\ &f_1(\theta) = \frac{1}{2} + \epsilon(12 - 48S^{-1}\theta). \end{aligned} \tag{53}$$

  Because $S^{-1}\theta = \left(6\epsilon\theta_1^2 + (1-6\epsilon)\theta_1\right)/2$, to first order in ϵ one eventually obtains:

$$f_1(\theta) = \frac{1}{2} + \epsilon(24\theta - 12). \tag{54}$$

- For $\theta \in [\frac{1}{2}, 1)$ the mapping (52) reads $\theta \to 2\theta + \epsilon\xi_2(\theta)$ and to first order in ϵ one obtains:

$$f_1(\theta) = \frac{1}{2} + \epsilon(24\theta - 12). \tag{55}$$

Combining the two contributions (54) and (55), we obtain the probability at time $t = 1$:

$$f_1(\theta) = 1 + 24\epsilon(2\theta - 1)\ , \quad \theta \in [0, 1). \tag{56}$$

As f_1 is our initial condition for the response function, we rename it f_0: $f_0(\theta) = 1 + 24\epsilon(2\theta - 1)$. Note that the mod 1 operation implies $S^t\theta = 2^t\theta - k$ with $k = 0, 1, ..., 2^t - 1$, if $\theta \in I_k = \left[\frac{k}{2^t}, \frac{k+1}{2^t}\right)$. Therefore, one can write

$$\Omega_{0,t}^{(k)}(\theta) = \log\frac{1 + 24\epsilon(2\theta - 1)}{1 + 24\epsilon[2(2^t\theta - k) - 1]} - t\log 2. \tag{57}$$

Restricted to I_k, the mapping is invertible at time t, so that $S^{-t}\theta = 2^{-t}(\theta + k)$ and:

$$\Omega_{0,t}^{(k)}(S^{-t}\theta) = \log\frac{1 + 24\epsilon(2\cdot 2^{-t}(\theta + k) - 1)}{1 + 24\epsilon(2\theta - 1)} - t\log 2. \tag{58}$$

Consequently, we have

$$\langle\theta\rangle_t = \int_0^1 d\theta\, f_0(\theta)\,\theta \sum_{k=0}^{2^t-1} e^{\Omega_{0,t}(S^{-t}\theta)} = 2^{-t}\int_0^1 d\theta\,\theta \left[2^t(1-24\epsilon) + \frac{48\epsilon}{2^t}\sum_{k=0}^{2^t-1}(\theta + k)\right] = \frac{1}{2} + \frac{4\epsilon}{2^t}, \tag{59}$$

which relaxes back exponentially rapidly to the unperturbed value, in accord with Eq. (12). Moreover, because this happens to all observables, and because the Ωt-mixing is necessary and sufficient for relaxation, this map has been proven to be Ωt-mixing.

V. 2. 1-dimensional contracting dynamics

For simplicity, consider first the second of Eqs.(8), and introduce $x = r - 1$, so that $x_{t+1} = x_t e^{-\mu}$. To show how Ω can be used to express the response, including the stable direction, let us start from a uniform distribution in [0,1]. Equation (44) then gives:

$$\langle x\rangle_t = \langle x e^{\Omega_{0,t}\circ S^{-t}}\rangle_0. \tag{60}$$

Trivially, we have $\Omega_{0,t} = \mu t$, while $\Omega_{0,t}\circ S^{-t}$ is a bit subtler:

$$\begin{aligned} \Omega_{0,t}\left(S^{-t}x\right) &= \mu t H(1 - S^{-t}x) = \\ &= \mu t H(S^t 1 - x) = \mu t H(e^{-\mu t} - x), \end{aligned} \tag{61}$$

where H is the Heaviside step function. Thus, we obtain the correct exponential decay:

$$\langle x\rangle_t = \int_0^{e^{-\mu t}} dx\, x e^{\mu t} = \frac{e^{-\mu t}}{2} = \langle x\rangle_0\, e^{-\mu t}. \tag{62}$$

Let us tackle more elaborate situations. Along the contracting direction, the authors of [1] take a Dirac delta, while our formalism requires that the initial distribution be regular. We can nevertheless compare our approach with that of Ref. [1] by introducing a smooth distribution function f on $(-\infty, +\infty)$, that approximates as closely as desired the Dirac measure at 0. The impulse perturbation at $t = 0$ yields:

$$f_0(x) = f(x - \delta x) \tag{63}$$

that, because of contraction in the stable direction, gets more and more concentrated under the time evolution, approximating better and better the perturbation of the singular measure of [1], while also relaxing toward the unperturbed singular measure. Actually, this is in line with Ruelle's approach, although that is limited to small perturbations of the steady state. In practice, let us take:

$$\mathrm{d}\mu(x) = f(x)\mathrm{d}x \quad \text{with} \quad f(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{x^2}{2\sigma^2}} \tag{64}$$

with small σ. Then, the dissipation function takes the following form:

$$\begin{aligned} \Omega_{0,t}(x) &= \Big[-\frac{x^2}{2\sigma^2}(1-e^{-2\mu}) + \mu \Big] t\,, \quad \text{and} \\ \Omega_{0,t}(S^{-t}x) &= \Big[-\frac{x^2 e^{-2\mu t}}{2\sigma^2}(1-e^{-2\mu}) + \mu \Big] t \end{aligned} \tag{65}$$

because $S^{-t}x = xe^{-\mu t}$. Substituting in Eq. (44) correctly yields:

$$\begin{aligned} \langle x \rangle_t = & \frac{1}{\sqrt{2\pi}\sigma} \int_{-\infty}^{\infty} dx e^{-\frac{x^2}{2\sigma^2}} \\ & \times x \Big[-\frac{x^2 e^{-2\mu t}}{2\sigma^2}(1-e^{-2\mu}) + \mu \Big] t = 0 \end{aligned} \tag{66}$$

since we are integrating an odd function over a symmetric domain about zero. Shifting the Gaussian to the right, to implement the perturbation, we have:

$$f_0(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-c)^2}{2\sigma^2}}, \quad c > 0 \tag{67}$$

$$\Omega_{0,t}(S^{-t}x) = -\frac{x^2}{2\sigma^2}(e^{2\mu t}-1) + \frac{cx}{\sigma^2}(e^{\mu t}-1) + \mu t \tag{68}$$

and, eventually,

$$\langle x \rangle_t = \frac{1}{\sqrt{2\pi}\sigma e^{-\mu t}} \int_{-\infty}^{\infty} dx\; x\; \exp\left\{ -\frac{(x-ce^{-\mu t})^2}{2\sigma^2 e^{-2\mu t}} \right\}. \tag{69}$$

Here, the time dependent distribution f_t is a Gaussian with moving mean $ce^{-\mu t}$ and shrinking variance $\sigma^2 e^{-2\mu t}$. In a realistic situation, in which there is a minimum scale δl that can be resolved, for an arbitrarily small ϵ, one can always choose a sufficiently small $\sigma(\delta l, \epsilon)$ such that

$$P_{0,c,\delta l/2} > 1-\epsilon, \quad P_{t,S^t c,\delta l/2} \doteq \int_{S^t c - \delta l/2}^{S^t c+\delta_l/2} dx f_{t,\sigma}(x). \tag{70}$$

Furthermore, if condition (70) is fulfilled at the initial time, it persists in time and it actually improves:

$$1 > P_{t+1,S^{t+1}c,\delta l/2} > P_{t,S^t c,\delta l/2} > 1-\epsilon, \; \forall t \in \mathbb{N}. \tag{71}$$

This means that a sufficiently sharp Gaussian is operatively equivalent to a Dirac's delta. Thus, we have re-derived the results (11) and (14) expressing the frequency dependent response to periodic forcing.

V. 3. 2-dimensional evolution

Let us combine the contracting and expanding dynamics of the previous sections, and let us take

$$\begin{aligned} & f_0(x,\theta) = [1+24\epsilon(2\theta-1)] \frac{1}{\sqrt{2\pi}\sigma} e^{\frac{(x-c)^2}{2\sigma^2}}, \\ & \text{and} \;\; \phi(x,\theta) = ax + b\theta. \end{aligned} \tag{72}$$

Observable ϕ lives in practice in a projected space of lower dimension than the phase space and, in a sense, mimics projections concerning thermodynamics. The dissipation function now takes the following form:

$$\begin{aligned} \Omega_{0,t}^{(k)}(x,\theta) &= \log \frac{1+24\epsilon[2\cdot 2^{-t}(\theta+k)-1]}{1+24\epsilon(2\theta-1)} - t\log 2 \\ + \mu t &- \frac{x^2}{2\sigma^2}(e^{2\mu t}-1) + \frac{cx}{\sigma^2}(e^{\mu t}-1). \end{aligned} \tag{73}$$

Then, substituting in (44), we obtain:

$$\begin{aligned} \langle \phi \rangle_t &= \Big\langle (ax+b\theta) \sum_{k=0}^{2^t-1} e^{\Omega_{0,t}^{(k)} \circ S^{-t} k} \Big\rangle_0 = \\ &= a\langle x \rangle_0 e^{-\mu t} + b\Big[\frac{1}{2} + 4\epsilon 2^{-t} \Big] = A + Be^{-\mu t} + C2^{-t}. \end{aligned} \tag{74}$$

This is the exact response, not limited to first order, for our observable in the projected space; it conveys information on the evolution of the initial ensemble f_0 while it relaxes to the singular invariant distribution. The constants A, B and C depend on the projection (a and b) and on the initial distribution f_0. We thus obtained the response in the projected space, which accounts for the responses along the unstable direction and along the stable direction.

Again, this relaxation implies that the dynamics under consideration is Ωt-mixing, because Ωt-mixing is necessary and sufficient for the relaxation of any initial ensemble.

V. 4. Convergence of single trajectories

The response (74) describes the ensemble behavior: on average the system relaxes to a stationary state with $\langle \phi \rangle_\infty$. The ergodicity of map (8) means that a time average over a single trajectory takes the same value with invariant probability 1. In this case, however, a set of zero phase space volume has unit probability. So standard ergodicity only speaks about a negligible fraction of the phase space. The fact that we can say more about (8) is due to its simple contracting mechanism, not to ergodicity.

To illustrate the single trajectory behavior, we performed simulations as in Ref. [1] for the cases of (49) and of (62), choosing a convergence tolerance of $\epsilon/2$ about $\langle \phi \rangle_\infty$, and calling convergence time $t_{c,\epsilon}$ the smallest time after which the time average remains within this tolerance. While in the unstable direction fluctuations due to (49) are large and for

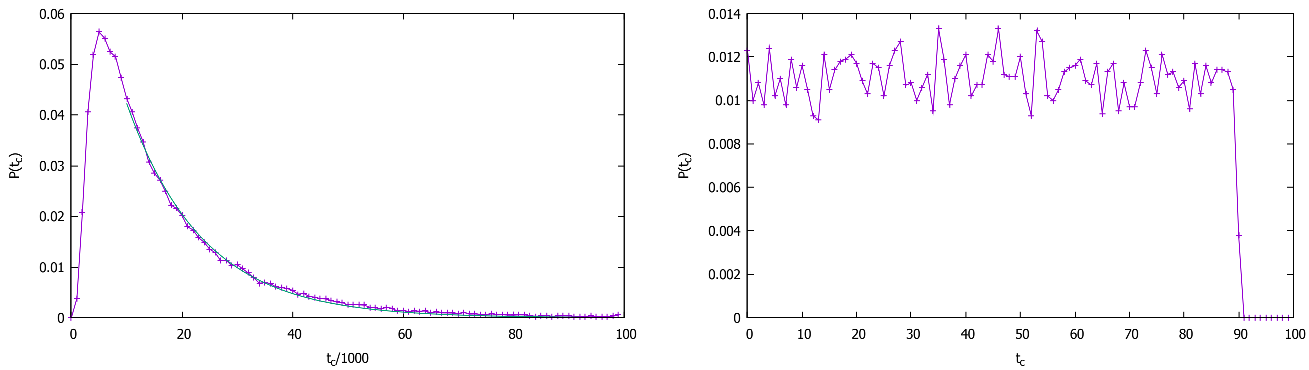

Fig. 1. Distribution of convergence times $t_{c,\epsilon}$ for $\epsilon = 0.01$. Left panel distribution concerns the unstable direction and is peaked about 5000 time steps (simulation with 10^5 samples). Almost indistinguishable from the data, the green line represents the exponential fit of the data in the tail of the distribution, showing that it decays exponentially. Right panel: distribution about stable direction is uniform like that in $[0, 1]$ of the initial conditions ($\mu = 0.2$; 10^4 samples)

$\epsilon = 0.01$ we have average $t_{c,\epsilon}$ of order $O(10^3) - O(10^4)$ time steps, in the stable direction (62) there are no fluctuations at all and convergence takes several steps, cf. Fig. 1. Combining the two, relatively large $t_{c,\epsilon}$ are obtained. As expected, the response in both directions amounts to relaxation toward the steady state for all initial conditions picked uniformly at random in the unit square. Exceptional trajectories such as unstable periodic orbits are indeed a set of zero volume, and are not found picking up at random. The dynamics (49) and (62) are thus not only Ωt-mixing, which is necessary and sufficient for ensemble relaxation, but they appear to be a good candidate for fully t-mixing dynamics [11, 12], because all single time averages, apart from those in a negligible volume, appear to converge to $\langle \phi \rangle_\infty$.

V. 5. Dissipative baker map

Consider the dissipative baker map defined as [32, 33]:

$$\begin{pmatrix} x_{t+1} \\ y_{t+1} \end{pmatrix} = S \begin{pmatrix} x_t \\ y_t \end{pmatrix} = \begin{cases} \begin{pmatrix} \frac{x_t}{l} \\ r y_t \end{pmatrix}, & x_t < l \\ \begin{pmatrix} \frac{(x_t - l)}{r} \\ r + l y_t \end{pmatrix}, & l \le x_t \le 1, \end{cases} \tag{75}$$

with $r = 1 - l$ and $l < r$; it is ergodic with probability density of the kind of Takagi functions [18]; it is invertible and it does not preserve phase space volumes locally [32, 33]. Although quite elementary, this map is more complicated than the previous ones, and the application of Ruelle's approach appears problematic, because of the effect of the discontinuity at $x = l$ on stable and unstable manifolds.

To investigate the evolution, we associate a string of t symbols with each trajectory of t steps, attributing symbol 0 to $x_k \le l$ (or $y_{k+1} \le r$) and symbol 1 to $x_k > l$ (or $y_{k+1} > r$), for all $k = 0, ..., t-1$. This allows us to to give an analytic expressions for S^t and S^{-t}. Moreover, symbol 0 implies phase space expansion and probability density lowered by the factor l/r, whereas symbol 1 implies phase space contraction and density increased by r/l. We call o_n the number of 1 in the string labelled by n, where $n = 0, ..., 2^t - 1$ ranges over all the possible strings. Then we have:

$$\begin{aligned} &\Omega_{0,t}(x) = \log \frac{f_0(x,y)}{f_0(S^t(x,y))} - \sum_{s=1}^{t} \Lambda(S^s(x,y)), \\ &\Lambda(x,y) = \begin{cases} \log(r/l), & x \le l \\ \log(l/r), & x > l \end{cases} \end{aligned} \tag{76}$$

and the response formula (44) gives:

$$\begin{aligned} \langle \mathcal{O} \rangle_t &= \left\langle \phi \, e^{\Omega_{0,t} \circ S^{-t}} \right\rangle_0 = \left\langle \sum_{n=0}^{2^t - 1} \chi_n \, \phi \, e^{\Omega_{0,t} \circ S^{-t}} \right\rangle_0 = \\ &= \left\langle \phi \sum_{n=0}^{2^t-1} \chi_n \frac{f_0 \circ S^{-t}}{f_0} \left(\frac{l}{r} \right)^{t - 2o_n} \right\rangle_0 , \end{aligned} \tag{77}$$

where f_0 is the initial ensemble and $\chi_n = 1$ in the set I_n of the initial conditions of trajectories of t steps labelled by n, and $\chi_n = 0$ elsewhere. While the border of I_n is $[0, 1]$ for every n in the x direction, they depend on n in the y direction. The numerical calculations (77) are shown in Fig. 2. The average of $\phi(x, y) = x$ is stationary if f_0 s uniform and it relaxes to the same value if f_0 is not uniform. For $\phi(x, y) = y$ the transient is more rapid and the convergence time and the steady state value do not depend on f_0. The slower relaxation for observable x is due to the fluctuations that are larger in the expanding direction than in the contracting one. As ensembles converge if and only if S is Ωt-mixing, this shows that S is indeed Ωt-mixing. To investigate the behavior of single trajectory time averages, we performed numerical simulations, as in section V. 4., with $\epsilon = 0.01$. Figures 3, 4 and 5 summarize the fact that for all initial conditions we could simulate convergence to the stationary state is reached for both

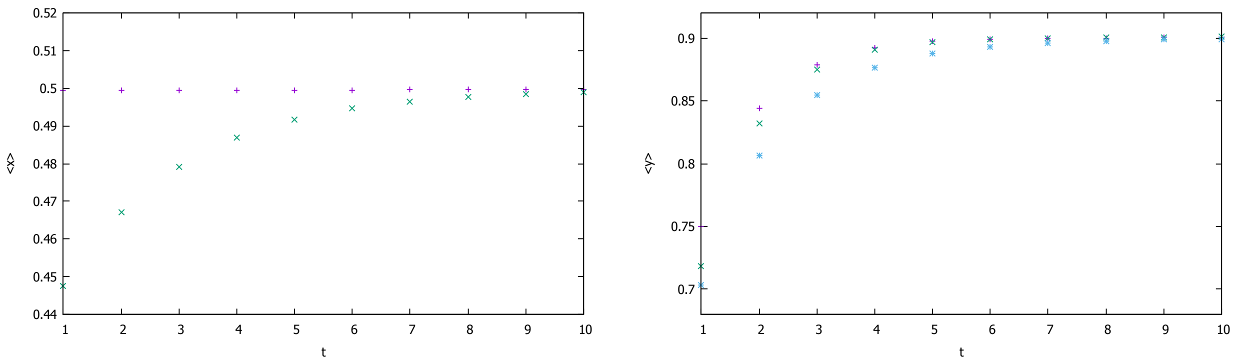

Fig. 2. Time dependent ensemble averages for the map of Eq. (75) from different initial ensembles. Left panel regards $\phi = x$: purple dots starting from a uniform distribution or linear in y, green crosses starting from a linear distribution in x; the stationary value is 0.5. Right panel regards $\phi(x, y) = y$: purple dots with uniform initial distribution, green crosses with initial distribution linear in y, blue stars distribution linear in x; the stationary value to which the initial ensambles converge is $\simeq 0.901$.

the observables, with a certain distribution of convergence times.[8]

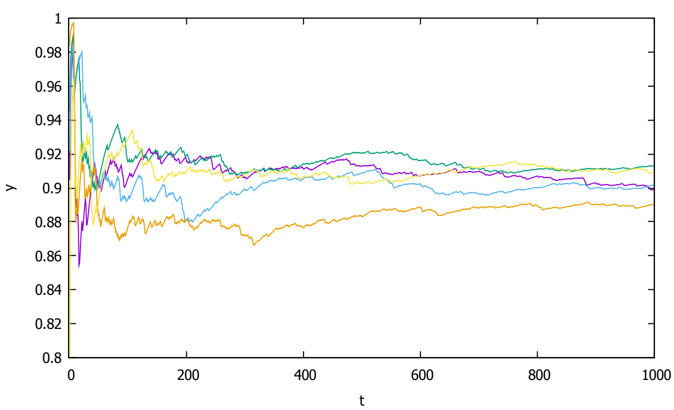

Fig. 3. Different behaviors of the quantity $\overline{y}(t)$ are shown for some random initial conditions in the unit square, evolving under the map (75). Initial fluctuations are quenched in time and all averages tend to $y_s \simeq 0.901$.

Analogously to the ensemble response, we observe that relaxation is slower for the observable x (peak of the distribution of $t_{c,\epsilon}$ around 9000 steps) than for the observable y (whose $t_{c,\epsilon}$ peaks around 1500 steps).

As the trajectories of the map S of Eq. (75) converge to a single steady state value no matter which initial condition one takes, S appears to be another possible candidate for the full t-mixing structure. Further, the heat-maps of Fig. 5, in which the initial conditions are plotted as functions of the corresponding convergence times show that this quantity is uniformly distributed in the unit square indicating that each portion of the phase space is statistically equivalent to the others, from this point of view. Note that the convergence time of the ensemble and the one of a trajectory must be interpreted in different ways. The first convergence time concerns a collection of objects, or a single system that is taken back exactly to the same statistical state after each measurement, for a number of times. The second can be computed performing a single measurement, on a time scale sufficient for the observable to explore the range of the relevant observables.

V. 6. Response for a non-ergodic map

Consider the following map, proposed in [31]:

$$\begin{pmatrix} x_{t+1} \\ y_{t+1} \end{pmatrix} = S \begin{pmatrix} x_t \\ y_t \end{pmatrix} = \\ = \begin{cases} \begin{pmatrix} \frac{1}{2} - \frac{1}{2} y_t \\ \frac{x_t}{2l} + \frac{1}{2} \end{pmatrix}, & 0 \leq x_t \leq l \\ \begin{pmatrix} 1 - 2l - (1-2l) y_t \\ \frac{x_t}{1-2l} - \frac{l}{1-2l} \end{pmatrix}, & l \leq x_t < \frac{1}{2} \\ \begin{pmatrix} 1 - \frac{1}{2} y_t \\ 2x_t - \frac{1}{2} \end{pmatrix}, & \frac{1}{2} \leq x_t < \frac{3}{4} \\ \begin{pmatrix} 1 - 2l y_t \\ 2x_t - \frac{3}{2} \end{pmatrix}, & \frac{3}{4} \leq x_t \leq 1. \end{cases} \tag{78}$$

There are different regimes depending on the value of l; we consider the ones with $\frac{1}{4} < l < \frac{1}{2}$. The stable and unstable directions, are more entangled than in the previous case. Map S is not time reversal invariant, however any trajectory segment of any number of steps t can be associated with one trajectory producing the opposite phase space volumes variation. Furthermore, for every trajectory segment there seems to be a different counterpart with opposite phase space contraction, for the different values of l.

Although this is not the standard situation, it suffices for the transient FR to be tested and for the general response formula (44) to be verified. To do that, we generalize the method used in section V. 5.. To each time step we associate a symbol from the alphabet $\{0, 1, 2, 3\}$, depending on which of the four regions of the unit square identified by Eq. (78)

[8] And thus this will also hold at least for their linear combinations, cf. Eq. (74).

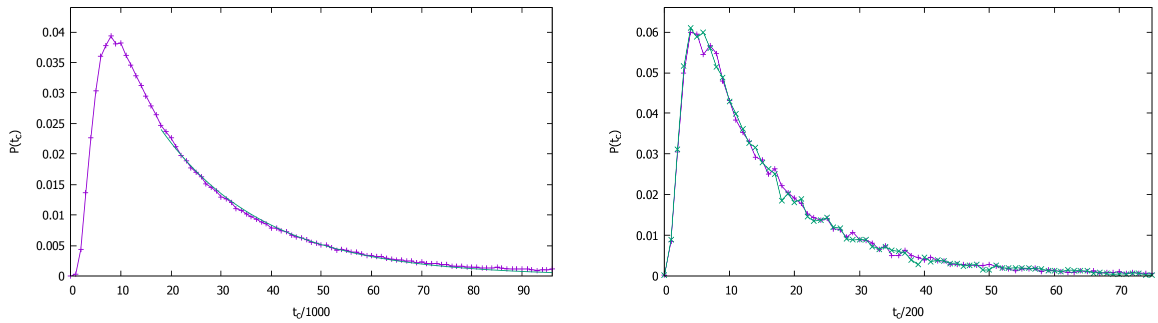

Fig. 4. Distributions of the convergence time $t_{c,\epsilon}$ for the map (75), with $\epsilon = 0.01$ and 10^6 samples. Left panel regards the observable $\phi(x, y) = x$: the peak is about 9000 time steps, larger than for the map (8). As in Fig. 1, the exponential fit of the tail (green line) is inditstinguishable from the data. Right panel is for the observable $\phi(x, y) = y$: purple dots represent convergence times for $\overline{y}$ computed starting at $t = 0$; green crosses starting after a transient of 1000 time steps. The two are equivalent, since after just ten time steps any initial ensamble converges to the stationary ensamble (cf. Fig. 2, right panel). After several time steps the statisticial properties coincide and do not change any more

the step starts. Unlike the dissipative baker map, not all transitions are allowed, here, but only the following ones: $0 \to 0$, $0 \to 1$, $1 \to 0$, $1 \to 1$, $1 \to 2$, $2 \to 2$, $2 \to 3$, $3 \to 2$, $3 \to 3$. Every trajectory of t steps is now associated with a string R of t symbols, which can be used to obtain an analitical expression for the time evolution S^t (or its inverse). Region 0 gets expanded and the probability density reduced by a factor $4l$. Region 3 is contracted and the probability density increased by a factor $1/4l$. The other two regions preserve volumes and densities. We call A_R the number of 0's and D_R the number of 3's in the string R. The response formula is then given by:

$$\langle \phi \rangle_t = \left\langle \phi \, e^{\Omega_{0,t} \circ S^{-t}} \right\rangle_0 = \left\langle \sum_{\{R\}} \chi_R \, \phi \, e^{\Omega_{0,t} \circ S^{-t}} \right\rangle_0 , \quad (79)$$

where the restriction of the dissipation function to a given R reads:

$$\Omega_{0,t}(S^{-t}(x, y)) = \\ = \log \frac{f_0(S^{-t}(x, y))}{f_0(x, y)} + (A_R(x, y) - D_R(x, y)) \log(4l). \quad (80)$$

Numerically evaluating Eq. (79), we find that ensemble relaxation to a steady state takes about thirty time steps (purple line in left panel of Fig. 6). Apart from the fact that ensemble relaxation is quite slower than for the dissipative baker map, here the crucial fact is that none of the averages computed numerically along single trajectories converges to that ensemble average. The map S is not ergodic: its phase space decomposes in various invariant regions, represented by different colors in the right panel of Fig. 6. Therefore, the time averages along single trajectories converge to four different values depending on their initial condition.

Therefore, the ensemble behavior does not describe the single system response, and this proves that this map is Ωt-mixing, with an asymptotic ensemble average that is the weighted mean (with respect to the initial distribution) of

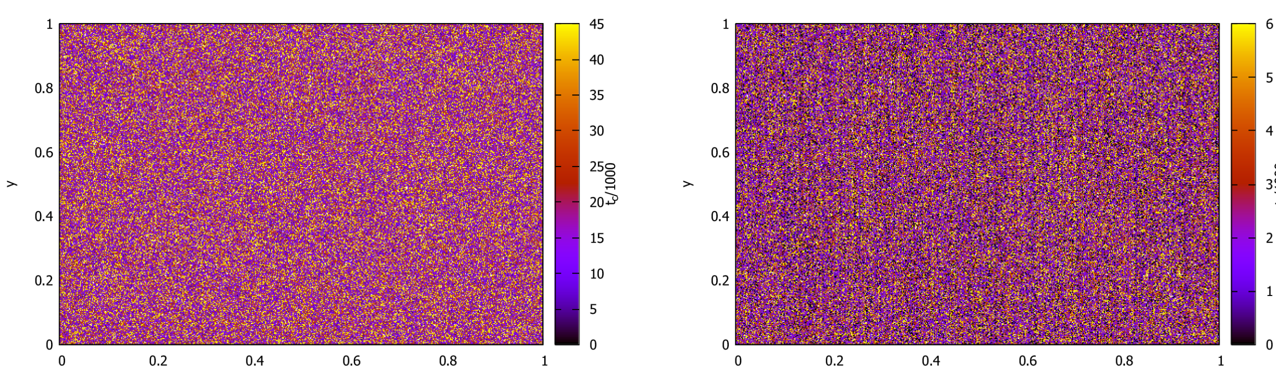

Fig. 5. Heat-maps for convergence times $t_{c,\epsilon}$ of map (75), with $\epsilon = 0.01$ and $5 \cdot 10^5$ samples. Each initial condition is colored depending on $t_{c,\epsilon}$ of the corresponding trajectory. The dominant color represents the peak in Fig. 4

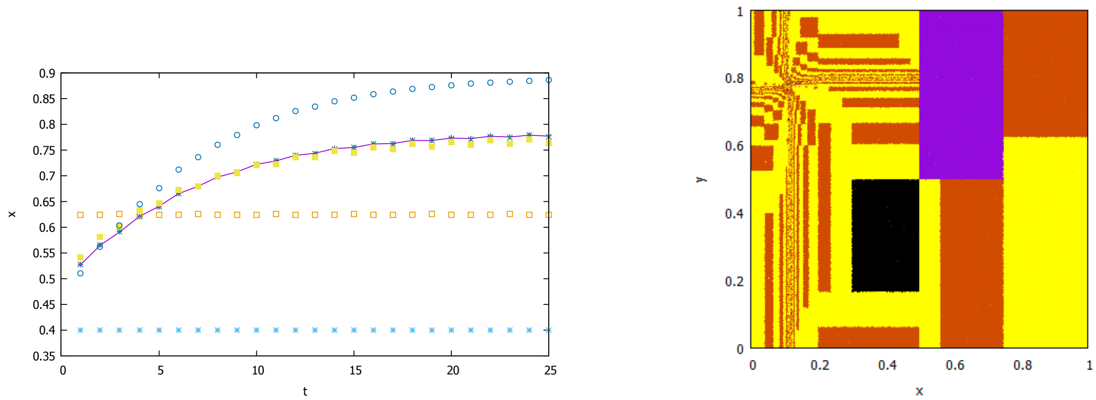

Fig. 6. Left panel: the purple line represents the ensamble response computed numerically from Eq. (79). Blue stars and orange squares are respectively the averages of initial conditions in the invariant sets B_{inv} and C_{inv}. Yellow squares refer to the average over trajectories converging to the period-four orbits $CDCD$; blue circles to trajectories converging to the fixed point P_D. The sum of these contributions gives the green crosses, in exact accord with the ensamble average. Right panel: Initial conditions colored according to the time average of each single trajectory (cf. left panel). In black and purple we have the invariant sets B_{inv} and C_{inv}. In orange and yellow we have the basins of attraction of the attractors $CDCD$ and P_D, including the fractal repeller

the four different averages, but it is not t-mixing. The right panel of Fig. 6, shows the interesting structure of the phase space of S, which consists of one attractor whose basin of attraction has a self similar structure that accumulates around one repeller, and invariant phase space volume preserving regions (see [31] for further details).

VI. CONCLUDING REMARKS

We have extended to time discrete dynamics the notions of physical ergodicity known as Ωt-mixing and t-mixing, developed for continuous time dynamics. For the first time we have identified systems that are Ωt-mixing, t-mixing and only Ωt-mixing, using the fact that Ωt-mixing is necessary and sufficient for ensemble relaxation [11, 12, 29]. When time averages over positive volumes of single trajectories converge to different values, despite the ensemble relaxation, the system is only Ωt-mixing, it cannot be t-mixing. We have illustrated these facts by means of exact solutions of simple (but even non-invertible) dynamical systems, and by direct simulations of the dynamics, to extract further quantitative information, such as the relaxation times for ensembles and single trajectories.

As in continuous time systems, the discrete time ensemble response theory, based on the Dissipation Function Ω, is general and not restricted to special kinds of dynamics. This generality implies that different Ωt-mixing situations may have different meanings, but there is no limitation to the use of the response formula. Analogously to the other response theories, Ωt-mixing expresses the average response of an ensemble of systems. Therefore, the single system response, that is also related to the issue of irreversibility [11, 12], must be deduced from other information. For instance, in absence of dissipation and for systems of very many weakly interacting constituents, one may rely on standard theories [34, 35]. However, the applicability of these theories is limited; for instance it excludes dissipative phenomena [12, 32]. t-mixing constitutes a sufficient condition for single systems relaxation [11, 12], but its relation with Ωt-mixing, that implies ensemble relaxation, needs to be investigated. In particular, the role of the number of degrees of freedom must be elucidated. The main features of this discrete time theory are those of the continuous time theory:

- the response of ϕ is given by the time correlation function of Ω and ϕ, with respect to the initial distribution f_0;
- the response formula is exact and not restricted to small perturbations;
- Ωt-mixing is necessary and sufficient for the relaxation of ensembles to a steady state;
- Ωt-mixing refers to a transient distribution and expresses the loss of macroscopic correlations;
- comparing with standard ergodicity and in relation to single systems relaxation, we note that ergodicity refers to sets of initial conditions of invariant probability 1, which in dissipative systems means sets of 0 phase space volume, negligible in the initial equilibria. t-mixing refers instead to the whole phase space, with 0-volume exceptions.

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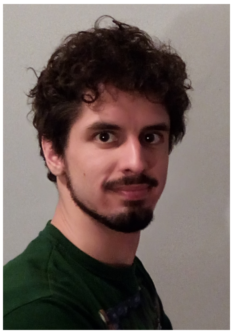

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