On the use of Ruelle's formalism in Response Theory

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Outline

- Ruelle's approach to Linear Response Theory
- Deterministic dynamics
    - Equilibrium
    - Dissipation
- Stochastic diffusions
    - Large Deviations approach
    - Detailed balance dynamics
    - Nonequilibrium steady states
- Nonlinear Response
- Conclusions

Let $(\mathcal{U}, S_o^t, \mu_o)$ be a dynamical system, with:

$\mathcal{U}$ a compact phase space, $S_o^t : \mathcal{U} \to \mathcal{U}$ a one-parameter group of diffeomorphisms, μ_o the invariant natural measure.

Assumption: the measure μ_o is absolutely continuous with respect to the Lebesgue measure:

$$\mu_o(dx) = \rho_o(x)dx \quad .$$

Let us add, at $t = 0$, a small perturbation $f_t(x) = h_t X(x)$, changing the dynamics into:

$$\dot{x}_t = \underbrace{F(x_t)}_{\substack{\textit{reference} \\ \textit{driving}}} + \underbrace{f_t(x_t)}_{\textit{perturbation}} \quad .$$

Following Ruelle, the response in a generic observable $Q : \mathcal{U} \to \mathbb{R}$ may be hence written as:

Ruelle's expansion

$$\langle Q(t) \rangle^h = \langle Q(t) \rangle^o + \sum_{n=1}^{\infty} \langle \delta Q(t) \rangle_n^h \quad ,$$

$\langle Q \rangle^h$ denotes the average of Q wrt the **perturbed** density, whereas $\langle Q(t) \rangle^o$ the average wrt the **unperturbed** density.

It holds:

$$\langle \delta Q(t) \rangle_n^h = \int_{-\infty}^{+\infty} ds_n ... \int_{-\infty}^{+\infty} ds_1 \, G^{(n)}(s_1, ..., s_n) h_{t-s_1} ... h_{t-s_n} \quad .$$

The n^{th} order Green function can be read off explicitly:

$$G^{(n)}(s_1, ..., s_n) = \int dx \rho_o(x)\theta(s_1)...\theta(s_n - s_{n-1}) \times \\ \times \mathcal{L}\mathcal{P}(s_n - s_{n-1})...\mathcal{L}\mathcal{P}(s_2 - s_1)\mathcal{L}\mathcal{P}(s_1)Q(x) \quad ,$$

with:

$$\mathcal{L}\Phi = X(x) \cdot \frac{\partial}{\partial x}\Phi$$

$$\mathcal{P}(t)\Phi = \Phi \circ S_o^t$$

At the linear order:

$$\langle \delta Q(t) \rangle_1^h = \int_0^{+\infty} G(t-s)h_s ds = \int_0^t R(t-s)h_s ds$$

where $R(t)$ is the Response function and $G(t) = \theta(t)R(t)$.

Thus, at the linear order, Ruelle's expansion yields the Fluctuation-Dissipation Theorem:

$$\begin{aligned}\langle \delta Q(t) \rangle_1^h &= \int_0^t h_s ds \int \rho_o(x_0) X(x_0) \left(\frac{\partial}{\partial x_0} Q(x_{t-s}) \right) dx_0 = \\ &= \int_0^t ds \int \sigma_s(x_s) Q(x_t) \rho_o(x_0) dx_0 = \langle S(\omega) Q(x_t) \rangle^o \quad ,\end{aligned}$$

where we introduced the *dissipative flux* $\sigma_s(x_s)$:

$$\sigma_s(x_s) = h_s \gamma(x_s)$$

with

$$\gamma(x) = -\frac{1}{\rho_o(x)} \left[\frac{\partial}{\partial x} \cdot (X(x) \rho_o(x)) \right] \quad .$$

$S(\omega)$ is the integral of σ_s over the path $\omega = (x_s, s \in [0, t])$.
For *conservative perturbations*, $S(\omega)$ corresponds to the Total Thermodynamic Entropy produced along the path.

Response function

$$R(t-s) = \langle \gamma(x_s) Q(x_t) \rangle^o$$

Two different contributions in $\sigma_s(x_s)$:

$$\sigma_s(x_s) = \underbrace{-\frac{\partial}{\partial x_s} \cdot f_s(x_s)}_{\sigma_A} + \underbrace{f_s(x_s) \cdot \frac{\partial}{\partial x_s}(-\log \rho_o(x_s))}_{\sigma_B} \quad . \qquad (1.1)$$

- σ_A is a dissipative contribution, triggered by nonconservative perturbations.
- σ_B is related to the work made by the perturbation (Kubo's theory).

Short digression on Fluctuation Relations

Let the involution G be defined as:

$$\frac{d(Gx)}{dt} = -f_t(Gx) \quad \rightarrow \quad D_G \cdot f_t = -f_t \circ G$$

with $G \circ G = 1$, and D_G denoting the Jacobian matrix of G.

$S(\omega)$ is odd under time reversal: $S(\omega) = -S(G\omega)$.

Fluctuation Relation for $S(\omega)$ (Evans & Morris, 1993):

$$\frac{\mathrm{Prob.}\left(S(\omega) \approx \overline{S}\right)}{\mathrm{Prob.}\left(S(G\omega) \approx -\overline{S}\right)} \approx \exp \overline{S}$$

Quantifies second law.

Obtained from theory of chaotic dynamical systems.

Related to ergodic theory by Gallavotti and Cohen (1995) who formulated the Chaotic Hypothesis.

Let the reference microscopic dynamics be Hamiltonian and the steady state be equipped with a density.

We add a small conservative perturbation, given by:

$$f_t(x) = h_t X(x) = -h_t S \frac{\partial V}{\partial x}$$

This corresponds to replacing the Hamiltonian $H_0(x)$ as:

$$H_0(x) \to H_0(x) - h_t V(x) \quad .$$

By taking, for simplicity: $\rho_o(x) = Z^{-1} \exp\left(-\beta H_0(x)\right)$, a straightforward calculation then yields:

- $\sigma_A = 0$
- $\sigma_s(x_s) = \sigma_B(x_s) = \beta h_s \frac{d}{ds} V(x_s)$

$$\langle \delta Q(t) \rangle_1^h = \beta \int \rho(x_0) dx_0 Q(x_t) \int_0^t ds \dot{V}(x_s) h_s$$

$$= \beta \int \rho(x_0) dx_0 Q(x_t) \left[\underbrace{(V(x_t)h_t - V(x_0)h_0) - \int_0^t ds V(s) \dot{h}_s}_{Heat} \right]$$

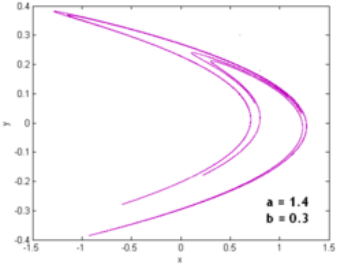
Note that:

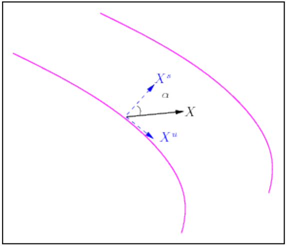
- $(V(x_t)h_t - V(x_0)h_0)$ is the extra change of energy in the environment due to the perturbation.
- $\int_0^t ds V(s) \dot{h}_s$ is the work done by the perturbation.

LRT is therefore cast as an equilibrium correlation between the observable and the Total Entropy produced along the path:

$$\langle \delta Q(t) \rangle_1^h = \beta \langle S(\omega) Q(x_t) \rangle^o \qquad R(t-s) = \beta \frac{d}{ds} \langle V(x_s) Q(x_t) \rangle^o$$

What happens when moving into Nonequilibrium?





Invariant measure μ_o is supported on a fractal attractor.

The standard FDT links the response to a perturbation to the statistical properties of the unperturbed system.

Not true, in general, in dissipative systems: the perturbed initial state and its time evolution may lie outside the support of μ_o.

Hence, their statistical properties cannot be expressed by μ_o, which attributes vanishing probability to such states.

For axiom A systems, Ruelle showed that the effect of a perturbation

$$f_t = f_t^{\|} + f_t^{\perp}$$

on the response of a generic (smooth enough) observable Q attains the form:

$$\langle \delta Q(t) \rangle_1^h = \int_0^t R_{\|}(t-\tau) f_\tau^{\|} d\tau + \underbrace{\int_0^t R_{\perp}(t-\tau) f_\tau^{\perp}(\tau) d\tau}_{\substack{extra \\ term}}$$

- $R_{\|}$ may be expressed in terms of a correlation function evaluated with respect to the unperturbed dynamics.
- $R_{\perp}$ depends on the dynamics along the stable manifold, hence it may not be determined by μ_o (and may also be quite difficult to compute numerically!).

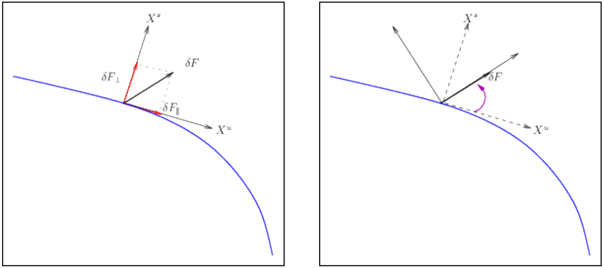


Figure: *Left panel*: In Ruelle's approach, the perturbation is expressed as the sum of one component parallel to the unstable manifold and one parallel to the stable manifold. *Right panel*: In our approach, the reference frame is rotated so that the direction of the perturbation coincides with one of the basis vectors.

Impulsive initial perturbation: $x_0 \to x_0 + \delta x_0$.

Linear Response:

$$\langle \delta x^i(t) \rangle_1^\delta = \int\int x_t^i \left[\rho_o(x_0 - \delta x_0) - \rho_o(x_0)\right] W(x_0, 0 \to x_t, t) dx_0 dx_t$$
$$= \left\langle x^i(t) \left(-\frac{\partial \log \rho(x_s)}{\partial x_s} \right) \right\rangle^o \cdot \delta x_0$$

Objection: the invariant measure μ of a dissipative system is singular (typically supported on a fractal attractor).
Thus, for dissipative systems the statistical features of a perturbation are not immediately related to the statistical properties of the unperturbed system: the perturbed initial state and its time evolution may lie outside the support of the invariant measure. Hence their statistical properties cannot be expressed by μ, which attributes vanishing probability to such states.

Alternative route to compute the response:

$$\langle \delta x^i(t) \rangle_1^{\delta} = \int x_t^i [\widetilde{\rho}_t(x^i; \delta x_0) - \widetilde{\rho}_o(x_t^i)] dx_t^i$$

where $\widetilde{\rho}_o(x_t^i)$ and $\widetilde{\rho}_t$ are the marginal probability distributions defined by:

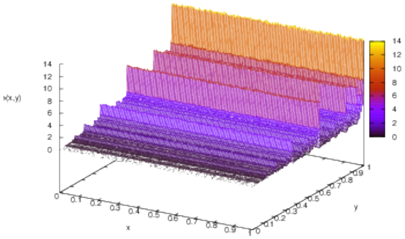
$$\widetilde{\rho}_o(x_t^i) = \int \rho_o(x_t) \prod_{j \neq i} dx_t^j \quad , \qquad \widetilde{\rho}_t(x_t^i; \delta x_0) = \int \rho_t(x_0; \delta x_0) \prod_{j \neq i} dx_t^j \quad .$$

Main message: projected singular measures are expected to be smooth, especially if the dimension of the projected space is sensibly smaller than that of the original space. In this case, the FDT can be extended to a considerable fraction of dissipative deterministic systems of interest in Physics.

Baker Map:
Let $\mathcal{M} = [0,1] \times [0,1]$ be the phase space, and consider the evolution equation

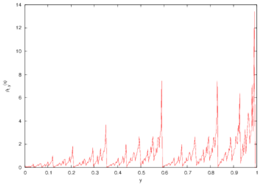
$$\begin{pmatrix} x_{n+1} \\ y_{n+1} \end{pmatrix} = M \begin{pmatrix} x_n \\ y_n \end{pmatrix} = \begin{cases} \begin{pmatrix} x_n/\ell \\ r y_n \end{pmatrix}, & \text{for } 0 \leq x_n < \ell; \\ \begin{pmatrix} (x_n - \ell)/r \\ r + \ell y_n \end{pmatrix}, & \text{for } \ell \leq x_n \leq 1. \end{cases} .$$

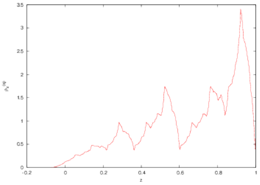
The map M is hyperbolic and dissipative for $\ell \neq 1/2$. It can also be shown that this dynamical system is endowed with an invariant measure μ which is smooth along the unstable manifold and singular along the stable one. In particular, μ factorizes as $\mathrm{d}\mu(x) = \mathrm{d}x \times \mathrm{d}\lambda(y)$.



Consider an initial impulsive perturbation and rotate the vectors of the basis so that the coordinate x lies along the direction of the perturbation. The projections of μ have a density along all directions except the vertical one.

A small perturbation does not take the state outside the corresponding projected support.





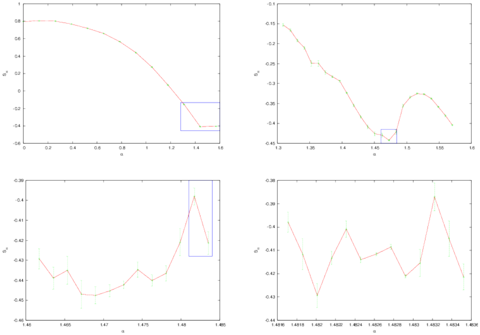
The Baker map shows that the response to very carefully selected perturbations, cannot be computed in general from solely the invariant measure.
However, the factorization of μ makes the present case rather peculiar. Indeed, for the overwhelming majority of dynamical systems, it looks impossible to select directions such that the projected measures preserve the same degree of singularity as the full measures. This is a consequence of the fact that stable and unstable manifolds have different orientations in different parts of the phase space, provided they exist. Clearly, the higher the dimensionality of the phase space and the larger the number of projected out dimensions, the more difficult it is to preserve singular characters.

Henon map:

$$\begin{pmatrix} x_{n+1} \\ y_{n+1} \end{pmatrix} = M \begin{pmatrix} x_n \\ y_n \end{pmatrix} = \begin{pmatrix} y_n + 1 - a x_n^2 \\ b x_n \end{pmatrix}$$

one the phase space $\mathcal{M} = [-\frac{3}{2}, \frac{3}{2}] \times [\frac{1}{2}, \frac{1}{2}]$, where $a = 1.4$ and $b = 0.3$ imply a chaotic dissipative dynamics, with a fractal invariant measure μ, which is not the product of the marginal measures obtained by projecting onto the horizontal and the vertical directions. These marginals are indeed regular and would yield a regular product.
As stable and unstable manifolds wind around, changing orientation, in a very complicated fashion, it seems impossible, here, to disentangle the contributions of one phase space direction from the other.

Because no direction appears to be priviledged in phase space, an initial perturbation along one of the axis should not lead to any singular perturbed projected measure, or irregular response function.

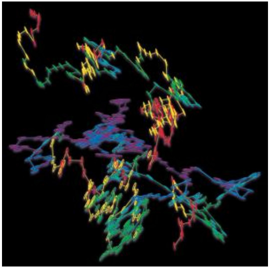


Shannon Entropy:

$$S_i = -\sum_q \rho_i^{(q)} \log(\rho_i^{(q)})$$

The presence of noise allows one to characterize the steady state, even in presence of dissipation, by regular probability densities.

On the other hand, the SRB measures constitute the zero noise limit of stochastically perturbed dynamical systems.



Extension of Ruelle's formalism to dynamical systems subjected to random perturbations.

We consider stochastic diffusions, described by the overdamped Langevin equations (inertial effects disregarded, forces proportional to velocities rather than to acceleration).

Definition

Overdamped Langevin equation for the state $x \in \mathbb{R}^n$

$$\dot{x}_t = \chi \cdot [F(x_t) + f_t(x_t)] + \nabla \cdot D(x_t) + \sqrt{2D(x_t)}\, \xi_t$$

with ξ_t = standard white noise.

The force F triggers the reference, unperturbed, dynamics:

$$F = F_{nc} - \nabla U$$

F_{nc} is a nonconservative force, U is the energy of the system.

- Path probability $P(\omega)$: paths starting from ρ_o and subjected to perturbation f_t.
- Path probability $P^o(\omega)$: paths starting from ρ_o and undergoing the reference dynamics.

$$P(\omega) = e^{-A(\omega)}\, P^o(\omega)$$

The action A may be split as: $A = (\mathcal{T} - S)/2$, with:

$$S(\omega) = A(G\omega) - A(\omega), \quad \mathcal{T}(\omega) = A(G\omega) + A(\omega)$$

General expression for $A(\omega)$ (Girsanov formula):

$$A(\omega) = \frac{\beta}{2}\int_0^t ds \left[f_s \cdot \chi F + \nabla \cdot (D f_s) + \frac{1}{2} f_s \cdot \chi f_s \right] - \frac{\beta}{2}\int_0^t \mathrm{d}x_s \circ f_s$$

with:

$$S(\omega) = \beta \underbrace{\int_0^t \mathrm{d}x_s \circ f_s}_{\text{work done by force}}, \quad \mathcal{T}(\omega) = \mathcal{T}_1 + \mathcal{T}_2$$

with

$$\mathcal{T}_1 = \beta \int_0^t ds \left[f_s \cdot \chi F + \nabla \cdot (D f_s) \right] \qquad \mathcal{T}_2 = \frac{\beta}{2}\int_0^t ds (f_s \cdot \chi f_s)$$

If the observable Q is even under the time-reversal, the following linear response holds:

$$\begin{aligned} \langle \delta Q(t) \rangle_1^h &= \langle Q(x_t) S(\omega) \rangle^o = - \langle Q(x_0) S(\omega) \rangle^o \\ &= - \int dx_0 \rho_o(x_0) Q(x_0) \langle S(\omega) \rangle_{x_0}^o \quad . \end{aligned}$$

which recovers the structure of the response formula obtained for deterministic systems. $\langle S \rangle_{x_0}^o$ denotes the conditional expectation of the entropy flux $S(\omega)$ over $[0, t]$ given that the path started from the state x_0. Its instantaneous flux is defined:

$$\langle S \rangle_{x_0}^o = \beta \int_0^t \langle w(x_s) \rangle_{x_0}^o ds$$

where $w(x_s)$ denotes to the instantaneous (random) work made by the perturbation f_t.

Let the reference dynamics be an equilibrium dynamics: $F_{nc} = 0$, i.e. $\rho_o(x) \propto e^{-\beta U(x)}$.

The quantity $w(x_s)$ pertaining to this stochastic dynamics can be explicitly computed:

$$w(x) = \frac{\chi}{\beta} \nabla \cdot f - \chi f \cdot \nabla U$$

From the knowledge of $w(x)$, one readily obtains the FDT for the stochastic process under consideration.

Alternatively, but equivalently, by computing $\sigma_s(x_s)$, one immediately recovers the expression for $\langle w(x_s) \rangle_{x_0}^{o}$.

It is also instructive to consider the case of a (conservative) perturbation changing the potential U into $U - h_t V$. For the case under consideration, the general response formula holds:

$$\begin{aligned} R(t-s) &= \frac{\beta}{2}\frac{d}{ds}\langle V(x_s)Q(x_t)\rangle^o - \frac{\beta}{2}\langle LV(x_s)Q(x_t)\rangle^o \\ &= -\beta\,\langle LV(x_s)Q(x_t)\rangle^o \end{aligned}$$

where L is the (backward) generator L of the process, defined as

$$L = -\chi\nabla U\cdot\nabla + \frac{\chi}{\beta}\nabla^2 \quad .$$

On the other hand, one also finds:

$$\gamma(x) = \beta\chi\nabla U\cdot\nabla V - \chi\nabla^2 V \quad . \tag{3.1}$$

which leads to the same FDT formula.

Definition

Fokker Planck equation

$$\frac{\partial \rho_t}{\partial t}(x_t) = -\nabla \cdot [\chi(F + f_t)\rho_t(x_t) - \frac{\chi}{\beta}\nabla \rho_t(x_t)]$$

If $F_{nc} \neq 0$ (e.g. friction) for the reference dynamics, the time-reversibility is broken (no detailed balance dynamics).

The NESS is characterized by an invariant density $\rho_o(x)$ (not know, in general).

In the steady state, one can define the information potential $\mathcal{I}_{\rho_o}$ as:

$$\mathcal{I}_{\rho_o} = -\frac{d \log \rho_o}{dx} = \frac{\beta}{\chi}u - \beta F$$

where $u \equiv j_{\rho_o}/\rho_o$ denotes a probability velocity.

General response function for overdamped diffusions:

$$R(t-s) = \chi \left\langle \left[-\frac{d}{dx_s} \cdot f(x_s) + \mathcal{I}_{\rho_o}(x_s) \cdot f(x_s) \right] Q(x_t) \right\rangle$$

If the perturbation has a gradient form $f = \nabla V$, the Response function attains the form:

$$R(t-s) = \underbrace{-\beta \left\langle \left(u(x_s) \cdot \nabla V(x_s) \right) Q(x_t) \right\rangle}_{\substack{\text{Nonequilibrium} \\ \text{correction}}} + \underbrace{\beta \frac{d}{ds} \left\langle V(x_s) Q(x_t) \right\rangle}_{\substack{\text{Equilibrium} \\ \text{Green-Kubo}}} \tag{3.2}$$

The equilibrium Kubo formula is reconstructed for $F_{nc} = 0$ (i.e. $u = 0$) or when describing the response in a reference frame moving with drift velocity u.

Going to second order:

$$\langle \delta Q\rangle_2^h(t) = \int_0^\infty ds_1 h_{t-s_1} \int_{s_1}^\infty ds_2 h_{t-s_2} \times$$
$$\times \int dx_0 \rho_o(x_0) \left[\gamma^{(2)}(x_0, x_{s_2-s_1}) + \chi^{(2)}(x_0, x_{s_2-s_1})\right] Q(x_{s_2})$$

where the second order terms $\gamma^{(2)}$ and $\chi^{(2)}$, are even the under time-reversal, and defined as:

$$\gamma^{(2)}(x_0, x_s) = \gamma(x_0)\gamma(x_s) \qquad \chi^{(2)}(x_0, x_s) = -X(x_s)\frac{\partial \gamma(x_0)}{\partial x_0} L^{-1}(s, x_0)$$

- $\gamma^{(2)}$ yields the leading non-vanishing correction to $\langle \sigma \rangle$.
- $\chi^{(2)}$ describes the coupling between the perturbation flow and the gradient of the dissipative flux through the tangent linear operator.

From the perspective of the large deviation approach, the role of time-symmetric quantities becomes also explicitly visible at the second order, where one has:

$$\langle \delta Q(t) \rangle_2^h = -\frac{1}{2} \langle Q(x_t) S(\omega) \mathcal{T}_1(\omega) \rangle^o$$

featuring the combined contribution of both the (linear order) time-symmetric and time-antisymmetric components of the action. It is not straightforward to establish a neat correspondence between our second order results and those pertaining to the large dev. approach.
Nevertheless, it is worth shedding light on the deterministic interpretation of the dynamical activity $\mathcal{T}$, whose role in statistical mechanics has been largely unnoticed so far.

- Response Theory formalism. A general framework was originally developed by Ruelle for axiom A systems.
- Deterministic systems. Equilibrium is well-known. In Nonequilibrium, difficulties stem from the lack of smoothness of the invariant measure.
- Stochastic dynamics. Noise allows one to introduce densities even in presence of dissipation. Our results allow to recover response formulae obtained by means of Large Deviations theory.
- Second order. Novel structures arises, not well understood yet. Some of them may be more concerned with kinetics than they are embedded into classical thermodynamics.

Some, very short, bibliography:

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