On a response formula and its interpretation

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Abstract: We present a physically inspired generalization of equilibrium response formulæ, the fluctuation-dissipation theorem, to Markov jump processes possibly describing interacting particle systems out-of-equilibrium, following the recent work of [1, 2]. Here, the time-dependent perturbation adding a potential $V$ with small amplitude $h_t$ changes the rates $W(x, y)$ for the transition $x \to y$ into

$$W_t(x, y) = W(x, y) e^{h_t(bV(y) - aV(x))}$$

as first considered by Diezemann, [4]; $a, b$ are constants. We observe that the linear response relation shows a reciprocity symmetry in the nonequilibrium stationary regime and we interpret the connection with dynamical fluctuation theory.

Dedicated to the 15th birthday of
Markov Processes and Related Fields.
1. Hurrah

The present paper is devoted to an important theme of statistical thermodynamics and system theory. It deals with the response of a system to an external stimulus. More specifically, we are interested in the linear response to an energy impulse applied to nonequilibrium systems and generalizing the celebrated fluctuation-dissipation theorem. That question comes up in the general construction of nonequilibrium statistical mechanics, but has possible applications in a variety of contexts. It is not clear yet whether the answer that we give here and that was presented in a more restricted sense in the physics literature \[1, 2\], is operationally useful. We do however attempt some interpretation directed towards dynamical fluctuation theory. The mathematical origin of all this is the theory of stochastic processes, here in its most simple representation for Markov jump processes on finite alphabets. The very fact that physically interesting relations can possibly be suggested already from the elementary mathematical theory of Markov processes is rather encouraging for the Markov field. That is then our contribution to the celebration of a young journal devoted to that subject, hurrah and many years to come.

2. Response in equilibrium

Relations between fluctuations, response behavior and dissipation in equilibrium systems have been obtained and applied throughout the development of statistical mechanics in the 20th century, \[7\]. Quite often textbooks treat linear response in a quantum mechanical context when applied to discrete systems such as spins or particles hopping on a lattice. The method for that equilibrium fluctuation-dissipation theorem is first order perturbation theory on time-dependent Liouville–von Neumann equations.

Here we consider stochastic evolutions, Markov jump processes; we give a more probabilistic treatment and corresponding statistical mechanical interpretation. The mathematics remains elementary.

2.1. Equilibrium dynamics. Let us consider a simple situation, which falls in the context of the present discussion. Take an Ising spin system on a finite graph \((\Lambda, \sim)\); at each vertex \(i \in \Lambda\) there is a spin \(\sigma(i) = \pm 1\). A spin flip Markov dynamics on the configurations \(\sigma \in \{+1, -1\}^\Lambda \equiv K\) has possible transitions \(\sigma \rightarrow \sigma^j\) where \(\sigma^j(i) = \sigma(i)\) for \(j \neq i\) and \(\sigma^j(j) = -\sigma(j)\) is the new configuration with the spin flipped at vertex \(j\). Physically, we imagine that there is a thermal reservoir perhaps in the form of lattice vibrations or of electronic degrees of freedom attached to the system so that for each transition \(\sigma \rightarrow \sigma^j\) there is an energy exchange \(U(\sigma^j) - U(\sigma)\) with and an entropy flux \([U(\sigma) - U(\sigma^j)]/T\) in the reservoir at equilibrium temperature \(T\). There is no need here
to specify that energy function $U(\sigma)$. As long as we assume the system is only in contact with the outside world through this one temperature bath, there should be a reversible stationary distribution $\rho$ giving probabilities

$$\rho(\sigma) = \frac{1}{Z} e^{-\beta U(\sigma)}$$

(1)

to the spin configurations. We call it the equilibrium distribution. The reversibility is expressed by the condition of detailed balance

$$W(\sigma, \sigma^j) \rho(\sigma) = W(\sigma^j, \sigma) \rho(\sigma^j), \quad \text{for all } j \in \Lambda, \sigma \in K$$

for the rates $W(\sigma, \sigma^j)$ of the transitions $\sigma \rightarrow \sigma^j$. Remark that all static properties of the system depend only on that part of the rates that is determined by the detailed balance condition. In other words, as long as the rates satisfy

$$\frac{W(\sigma, \sigma^j)}{W(\sigma^j, \sigma)} = e^{-\beta [U(\sigma^j) - U(\sigma)]}$$

they will simulate the correct physical properties of the system. Explicitly, the transition rates of the stochastic Ising model are

$$W(\sigma, \sigma^j) = \psi(\sigma, j) \exp \left( -\frac{\beta}{2} [U(\sigma^j) - U(\sigma)] \right)$$

(2)

and all produce the same equilibrium \([\text{1}]\) independent of the prefactor $\psi(\sigma, j) = \psi(\sigma^j, j)$ as long as it indeed does not depend on $\sigma(j)$. Moreover there is then a time-reversal symmetry for the stationary process: denoting by $P_\rho$ the stationary Markov (equilibrium) process with stationary law $\rho$, we have equilibrium correlations

$$\langle f(\sigma_s) g(\sigma_t) \rangle_{\text{eq}} = \langle f(\sigma_t) g(\sigma_s) \rangle_{\text{eq}}$$

(3)

which are functions of $|t - s|$. The brackets $\langle \cdot \rangle_{\text{eq}}$ denote an average over the equilibrium ensemble over all possible realizations of the stochastic process determined by \([\text{1}] - \text{[2]}\).

2.2. Perturbation and response. Suppose now that we start in equilibrium $\rho$ at time $t = 0$ but thereafter we slightly modify the dynamics in a time-dependent way. For times $s \in [0, t]$ we switch on a magnetic field of small amplitude $h_s$. That is the external stimulus by which we change the energy function $U$ into $U - h_s V$ for $V(\sigma) = \sum_{i \in \Lambda} \sigma_i$. How will the equilibrium system respond at time $t > s$, and does the choice of $\psi$ in the rates \([\text{2}]\) make a difference?

We look at the linear response

$$\langle Q(t) \rangle_{\rho}^h = \langle Q(t) \rangle_{\text{eq}} + \int_0^t ds \, h_s R^\text{eq}_{QV}(t, s) + o(h)$$

Here, $Q(t) = Q(\sigma_t)$ is a function of the random spin configuration evaluated at time $t > 0$. The left-hand side averages over the perturbed dynamics, depending on the $h_s$, and over the initial equilibrium $\rho$; the
right-hand side averages over the unperturbed dynamics always starting in \( \rho \): \[ \langle Q(t) \rangle_{eq} = \sum_{\sigma} \rho(\sigma) Q(\sigma) \] as the equilibrium is time-invariant. The linear correction contains the response function or generalized susceptibility \( R^\text{eq}_{QV}(t, s) \) which is our object of study. Formally and leaving away further decorations,

\[ R_{QV}(t, s) = \frac{\delta}{\delta h_{\sigma}} \bigg|_{h=0} \langle Q(t) \rangle^h \]

An interesting case looks at the response in the magnetization itself, taking \( Q = V = \sum \sigma(i) \) and then

\[ R^\text{eq}_{QV}(t, s) = \beta \sum_{i,j \in \Lambda} \frac{\partial}{\partial s} \langle \sigma_s(i) \sigma_t(j) \rangle_{eq}, \quad 0 < s < t \quad (4) \]

is expressible as a space-time–correlation function in the equilibrium process. That formula is valid for all times \( 0 < s < t \) and for all choices of rates that satisfy detailed balance. It is an example of the fluctuation-dissipation theorem for finite-time perturbations. The more general equilibrium formula of which \( (4) \) is a special case reads

\[ R^\text{eq}_{QV}(t, s) = \beta \frac{\partial}{\partial s} \langle V(s) Q(t) \rangle_{eq}, \quad 0 < s < t \quad (5) \]

which is again true for any choice \( (2) \) of the rates that satisfies detailed balance. A proof of this is easy by applying first-order time-dependent perturbation theory and by inserting the equilibrium condition \( (1) \).

If we integrate \( (1) \) over \( s \in [0, t] \) with constant \( h_s = h \), then

\[ \langle Q(t) \rangle^h - \langle Q(t) \rangle_{eq} = h\beta[\langle V(t) Q(t) \rangle_{eq} - \langle V(0) Q(t) \rangle_{eq}] \quad (6) \]

Taking \( t \uparrow +\infty \) we recognize the usual change in the equilibrium Boltzmann-factor to first order in \( h \) when changing the potential \( U \rightarrow U - hV \).

The conclusion in equilibrium: adding a potential to a system with an equilibrium dynamics is unambiguous, at least when looking at linear response and there is a simple and explicit linear response formula in terms of an equilibrium correlation in which we recognize the Boltzmann factor.

The rest of this paper addresses the question what happens if the unperturbed dynamics is out-of-equilibrium. The answer is again an explicit formula (see \( (12) - (20) \) below) but the choice of how to add a potential now does have some influence on the response formula. Moreover, there is an interesting interpretation of the resulting correlations in terms of dynamical fluctuations, which extends equilibrium considerations — see Proposition \( 3 \).
3. Going nonequilibrium

The extension of the previous problem to a nonequilibrium set-up has been considered in many papers. We take here the approach of [1, 2].

We consider a Markov stochastic dynamics for a finite system. Denote the state space by $K$. We have transition rates $W(x, y), x, y \in K$. We do no longer assume that there is a potential, i.e. a function $U(x), x \in K$ for which $W(x, y) \exp -U(x) = W(y, x) \exp -U(y)$. In particular, for a stationary distribution $\rho(x), x \in K$, while

$$
\sum_{y \in K} [\rho(x) W(x, y) - \rho(y) W(y, x)] = 0, \quad x \in K
$$

still, there are nonzero currents of the form $\rho(x) W(x, y) - \rho(y) W(y, x) \neq 0$ for some pairs $x \neq y \in K$. The stationary process (Markov dynamics in $\rho$) is then no longer time-reversible. We have in mind systems of stochastically interacting particles which are driven away from equilibrium; the state $x$ is then the total configuration of particles and the transitions are local. An example follows in Section 5.

Secondly, we also do not need to assume that we start at time $t = 0$ from a stationary distribution. Rather, we have an arbitrary probability distribution $\mu(x), x \in K$, from which the initial data are drawn and then for $t > 0$ we apply the perturbed dynamics.

The question is first how to perturb the transition rates $W(x, y) \rightarrow W_t(x, y)$, by adding an extra potential $-h_t V$ to the system. For convenience we assume that the perturbation $h_s, s > 0$, is twice differentiable. Our (physical) assumption here is that the perturbed rates at time $t > 0$ should satisfy

$$
\frac{W_t(x, y)}{W_t(y, x)} = \frac{W(x, y)}{W(y, x)} e^{\beta h_t [V(y)-V(x)]}
$$

(7)

The inverse temperature $\beta$ signals that the perturbation concerns an additional energy exchange with a reservoir at temperature $\beta^{-1}$. The assumption (7) is conform the condition of local detailed balance as often applied in particle systems. That is why we speak of an energy impulse.

Condition (7) leaves many possible choices for the perturbed transition rates. A quite general choice is

$$
W_t(x, y) = W(x, y) e^{h_t [bV(y)-aV(x)]}
$$

(8)

where the $a, b \in \mathbb{R}$ are independent of the potential $V$; it was considered in [4]. To satisfy (7) we need that $a + b = \beta$ but $a$ or $b$ can still vary. A first choice is

$$
W_t^{(1)}(x, y) = W(x, y) e^{\frac{4h_t}{2} [V(y)-V(x)]}
$$

(9)
in which case $a = b = \beta/2$; that is sometimes called the force-model and was explicitly treated in [2]. A second case is

$$W_t^{(2)}(x, y) = W(x, y) e^{-\beta h_t V(x)}$$

whence $b = 0, a = \beta$, or the opposite $b = \beta, a = 0$.

It is instructive to understand the difference between these cases: we can rewrite (8) as

$$W_t(x, y) = W(x, y) e^{h_t \frac{b-a}{2}[V(y)+V(x)]} e^{\frac{h_t a}{2}[V(y)-V(x)]}$$

and we see that making $a \neq b$ gives an extra $x \leftrightarrow y$ symmetric but time-dependent prefactor $\psi_t(x, y) = \psi_t(y, x) = \exp h_t \frac{b-a}{2}(V(y)+V(x))$ with respect to the force-model of (9). Visualizing the situation in terms of a one-dimensional potential landscape we imagine the states $x$ located at the local minima of a potential $U$ and separated from each other via energy barriers. The Arrhenius formula then predicts a rate $W(x, y) \propto \exp -\beta[D(x, y) - U(x)]$ where $D(x, y) = D(y, x)$ is the barrier height between states $x$ and $y$. Naturally, adding a time-dependent potential landscape can affect both the symmetric prefactor $D(x, y)$ and the local minima $U(x)$ themselves which gives a possible interpretation of the two constants $a$ and $b$. For example, choosing (10) only changes the depth of the local minima (binding energies $U(x) \to U(x) - h_t V(x)$) and not the barrier heights. The above picture works best under equilibrium conditions, but one now imagines that the nonequilibrium driving adds further asymmetries.

The linear response question remains unchanged: at time $t > 0$ the expected value of an observable $Q$ will probably deviate from the expectation under the unperturbed dynamics. Linear response theory out-of-equilibrium is interested in estimating and interpreting the deviations

$$\langle Q(t) \rangle^h_\mu - \langle Q(t) \rangle^\mu$$

to first order in $h$. We have abbreviated $Q(t) = Q(x_t)$ for the observable at time $t$. In other words, we want to compute $R_{QV}^\mu(t, s) = R(t, s), 0 < s < t$, in

$$\langle Q(t) \rangle^h_\mu = \langle Q(t) \rangle^\mu + \int_0^t ds \, h_s R(t, s) + o(h)$$
4. Response formula

The present section computes the response function \( R(t, s) \) for the general perturbation of the form (8). In the formula appears the backward generator \( L \) of the jump process; in terms of the transition rates,

\[
Lf(x) = \left. \frac{d}{ds} \right|_{s=0} \langle f(x_s) \rangle_{x_0=x} = \sum_y W(x, y) [f(y) - f(x)]
\]

**Proposition 1.** For a perturbation of the form (8), the response function is equal to

\[
R(t, s) = b \frac{\partial}{\partial s} \langle V(x_s) Q(x_t) \rangle_\mu - a \frac{\partial}{\partial t} \langle V(x_s) Q(x_t) \rangle_\mu + b \left[ \langle V(x_s) LQ(x_t) \rangle_\mu - \langle LV(x_s) Q(x_t) \rangle_\mu \right] \tag{12}
\]

The proof of this result is essentially a linear order perturbation of the Girsanov-formula for the density of the perturbed versus the original path-space measures.

**Proof of Proposition 1.** To see where we must go, we first rewrite the right-hand side of (12). In particular, the third term involving \( LQ \) can directly be combined with the second term, time-derivative in \( t \), adding up to \((b - a)\) multiplied with

\[
\frac{\partial}{\partial t} \langle V(x_s) Q(x_t) \rangle_\mu = -\frac{\partial}{\partial s} \langle V(x_s) Q(x_t) \rangle_\mu + \sum_x \mu_s(x) V(x) e^{(t-s)LQ(x)}
\]

where \( \mu_s(x) = \sum_y W(y, x) \mu_s(y) - \sum_y W(x, y) \mu_s(x) \) solves the master equation starting from \( \mu_0 = \mu \). As a consequence, we really must prove that

\[
R(t, s) = a \frac{\partial}{\partial s} \langle V(x_s) Q(x_t) \rangle_\mu - b \langle LV(x_s) Q(x_t) \rangle_\mu - (b - a) \sum_y \langle W(x_s, y) V(x_s) Q(x_t) \rangle_\mu \tag{13}
\]

\[
+ \quad (b - a) \sum_{x, y} \mu_s(y) W(y, x) V(x) e^{(t-s)LQ(x)}
\]

Let a path be denoted by \( \omega = (x_s)_s, s \in [0, t] \), for \( x_s \in K \). Paths are piecewise constant and chosen with left limits and right continuous at every jump time. For the perturbed process

\[
\langle Q(t) \rangle_\mu^h = \int dP_\mu(\omega) \frac{dP_\mu^h}{dP_\mu}(\omega) Q(x_t)
\]

where we have inserted the density between the path-measures \( P_\mu^h(\omega) \) for the perturbed and the unperturbed \((h = 0)\) Markov dynamics starting from law \( \mu \) at time zero. Explicitly (see e.g. Appendix 2 in [6]),
the Girsanov formula gives
\[
\log \frac{dP^h_\mu}{dP_\mu}(\omega) = \sum_{s \leq t} h_s [bV(x_s) - aV(x_{s-})] \\
- \sum_y \int_0^t ds \, W(x_s, y) \left[ e^{h_s [bV(y) - aV(x_s)]} - 1 \right]
\] (15)

where the first sum is over all the jump times \( s \in [0, t] \). Up to linear order in \( h \), and with some reordering of the terms, this becomes
\[
\log \frac{dP^h_\mu}{dP_\mu}(\omega) = (b - a) \sum_{s \leq t} h_s V(x_s) + a \sum_{s \leq t} h_s [V(x_s) - V(x_{s-})] \\
- b \int_0^t ds \, h_s LV(x_s) - (b - a) \int_0^t ds \, h_s \sum_y W(x_s, y)V(x_s)
\] (16)

Higher order in \( h \) can easily be controlled. Its second term on the right still allows a partial summation into
\[
\sum_{s \leq t} h_s [V(x_s) - V(x_{s-})] = h_t V(x_t) - h_0 V(x_0) - \sum_{s \leq t} V(x_{s-}) \left[ h_s - h_{s-} \right]
\]
\[
= h_t V(x_t) - h_0 V(x_0) - \int_0^t ds \, \frac{d}{ds} h_s \, V(x_s)
\] (17)

The expression (16) must now be multiplied with \( Q(x_t) \) and averaged over the original Markov process starting from \( \mu \), after which we note that
\[
\langle \{ h_t V(x_t) - h_0 V(x_0) \} - \int_0^t ds \, \frac{d}{ds} h_s \, V(x_s) \rangle Q(x_t)_\mu = \int_0^t ds \, h_s \frac{\partial}{\partial s} \langle V_s Q_t \rangle_\mu
\] (18)

reproduces the first term in (13). The last two terms in (16) are also easily identified giving rise to the two middle terms in (13). That leaves us with the very first term in (16) for which must hold that
\[
\langle \sum_{s \leq t} h_s V(x_s) Q(x_t) \rangle_\mu = \sum_{x,y} \int_0^t ds \, h_s \mu_s(y)W(y, x) V(x)e^{(t-s)L}Q(x)
\]

That is indeed true as can be seen by writing the sum over all jump times in terms of the random measure \( dk_s(y, x) \) on paths \( \omega \), which gives 1 when there is a jump \( y \to x \) at time \( s \), and is zero otherwise:
\[
\langle \sum_{s \leq t} h_s V(x_s) Q(x_t) \rangle_\mu = \sum_{x,y} V(x) \int_0^t h_s \langle dk_s(y, x) Q(x_t) \rangle_\mu
\]

By the Markov property \( e^{(t-s)L}Q(x) = \langle Q(x_t) | x_s = x, x_{s-} = y \rangle_\mu \) and
\[
\langle dk_s(y, x) Q(x_t) \rangle_\mu = \mu_s(y)W(y, x)e^{(t-s)L}Q(x) \, ds
\]
so that the conclusion \((12)\) is reached.

5. Example

We come back to the example \((2)\) of a purely dissipative spin-flip dynamics. We now add a mixing dynamics. More specifically, we not only have transitions \(\sigma \rightarrow \sigma^j\) with corresponding rates \(W(\sigma, \sigma^j)\), but now we also allow transitions \(\sigma \rightarrow \sigma^{ij}\) where the spins at neighboring vertices \(i \sim j \in \Lambda\) get exchanged: \(\sigma^{ij}(k) = \sigma(k)\), if \(i \neq k \neq j\) while \(\sigma^{ij}(i) = \sigma(j), \sigma^{ij}(j) = \sigma(i)\). The rate for these exchanges is \(\lambda > 0\). The result is a reaction-diffusion process on \(K = \{+1, -1\}^\Lambda\) with generator \(L\) acting on functions \(f : K \rightarrow \mathbb{R}\),

\[
Lf(\sigma) = \sum_{j \in \Lambda} W(\sigma, \sigma^j)[f(\sigma^j) - f(\sigma)] + \lambda \sum_{i \sim j}[f(\sigma^{ij}) - f(\sigma)]
\]

That unperturbed dynamics does not satisfy the condition of detailed balance when \(\beta \neq 0\) for a nontrivial energy function \(U(\sigma)\) in \((2)\). There is a stationary distribution \(\rho\) of which very little is known; in particular it can depend on the \(\psi\) in \((2)\).

We still consider the magnetization \(V(\sigma) = Q(\sigma) = \sum_i \sigma_i\) for organizing and evaluating the perturbation of amplitude \(h, t > 0\). Note that \(V(\sigma^{ij}) = V(\sigma)\) and the transition \(\sigma \rightarrow \sigma^{ij}\) leaves the total magnetization unchanged. Hence \(LV(\sigma) = -2 \sum_i \sigma_i W(\sigma, \sigma^i)\) is still the dissipation of magnetization due to the spin flip reaction. Let us abbreviate \(J_i(\sigma) = -2\sigma(i) W(\sigma, \sigma^i)\) for the systematic rate of change in the local magnetization. We get the linear response around steady nonequilibrium from \((12)\):

\[
\frac{\partial}{\partial h_s(i)} \left|_{h=0} \right. \langle \sigma_t(j) \rangle^h_{\rho} = a \frac{\partial}{\partial s} \langle \sigma_s(i) \sigma_t(j) \rangle_{\rho} - b \langle J_i(\sigma_s) \sigma_t(j) \rangle_{\rho}
\]

We see that the equilibrium expression \((1)\) gets modified by the correlation between \(\sigma_t(j)\) and the flux \(J_i(\sigma_s)\). For a constant perturbation \(h_s = h, s \in [0, t]\), we can integrate over \(s \in [0, t]\) to get the leading order of the response:

\[
\frac{1}{h} \sum_i \langle \sigma_t(i) \rangle^h_{\rho} - \langle \sigma_0(i) \rangle_{\rho} = a \sum_{i,j \in \Lambda} \langle [\sigma_t(i) - \sigma_0(i)] \sigma_t(j) \rangle_{\rho} - b \sum_{i,j \in \Lambda} \int_0^t ds \langle J_i(\sigma_0) \sigma_s(j) \rangle_{\rho}
\]

(19)

Note that the rate \(\lambda\) is hiding in the correlation functions but the form \((19)\) is unchanged no matter what is \(\lambda\).

The example is a more microscopic version of a reaction-diffusion model but it can also be considered as a toy model for a granular lattice gas undergoing inelastic collisions. The spins refer then to the presence or absence of energy packets which diffuse but can also be created or
get lost. The latter specifies the temperature of the environment and the flux $J_i$ in the above would be the systematic rate of local energy change.

6. More symmetries

In a number of cases the response formula (12) simplifies. There is first the case where the initial distribution is the stationary measure $\rho$. Then, i.e., when $\mu = \rho$ is the stationary distribution, correlation functions like $\langle V(x_s)Q(x_t) \rangle_\rho$ are functions of $t - s$, so that the response function becomes

$$R_{QV}(t, s) = a \frac{\partial}{\partial s} \langle V(x_s)Q(x_t) \rangle_\rho - b \langle L V(x_s)Q(x_t) \rangle_\rho$$

(20)

In equilibrium, i.e., under time-reversal symmetry, the two terms in the right-hand side of (20) coincide and we recover (5) whenever $a + b = \beta$ (and independent of $\psi$ in (2)).

For the case (9), this means that $b = a = \frac{\beta}{2}$, the response formula becomes

$$R_{QV}(t, s) = \frac{\beta}{2} \frac{\partial}{\partial s} \langle V(x_s)Q(x_t) \rangle_\mu - \frac{\beta}{2} \langle L V(x_s)Q(x_t) \rangle_\mu$$

which is in exact agreement with [1].

A special case arises when $b = 0$ and $a = \beta$ in (8), because then the response is of the same form as in equilibrium:

$$R(t, s) = -\beta \frac{\partial}{\partial t} \langle V(x_s)Q(x_t) \rangle_\mu$$

This is indeed a special kind of perturbation, as can also be seen from the following consideration. Take $h$ to be constant; the law $\rho^h$ defined by $\rho^h(x) \propto \rho(x) e^{hV(x)}$ is stationary for the new dynamics (to all orders in $h$). In other words, here the resulting behavior under this perturbation is like in equilibrium, even though the unperturbed dynamics can be far from equilibrium.

That last remark brings us to considering the limit $t \uparrow \infty$ of (12) in which the response formula should show stationary response. Imagine thus that we apply a new time-independent dynamics with rates

$$W^V(x, y) = W(x, y) e^{h[bV(y) - aV(x)]}, \text{ small constant } h$$

(21)

We assume that both the original ($h = 0$) and the perturbed dynamics show exponential ergodicity in converging to $\rho$, respectively $\rho^V$. Similarly we can replace in the above the function $V$ by another function $M$ on $K$ and construct $\rho^M$. Both $\rho^V$ and $\rho^M$ depend on $h$ and we investigate their change with respect to the original $\rho$ to first
order in $h$. The original backward generator is still $L$. The following proposition looks at a special observable, and we write

$$\chi_{MV}^{ab} = \frac{\delta}{\delta h} \bigg|_{h=0} \sum_x \rho^V(x) L M(x); \quad \chi_{VM}^{ab} = \frac{\delta}{\delta h} \bigg|_{h=0} \sum_x \rho^M(x) L V(x)$$

The dependence on the constants $a, b, h$ is not made explicit but sits in the perturbed dynamics, as in (21) for perturbing potential $V$ and similarly for perturbation $M$.

**Proposition 2.** The stationary response functions (22) equal

$$\chi_{MV}^{ab} = \chi_{VM}^{ba} = b\langle M L V \rangle_\rho + a\langle V L M \rangle_\rho$$

Observe the symmetry when interchanging $M$ and $V$ together with the exchange of $a$ and $b$. If the perturbation is of the form (9), then only interchanging $M$ and $V$ is enough. This symmetry appears useful because it reduces the amount of response functions to be measured. Moreover, some experimentally difficult responses can be made more accessible by interchanging the role of observable and perturbation.

While its proof is trivial, we are not aware that this symmetry (23) has been observed before. On the level of generators it simply amounts to the direct observation that

$$(L^V_{ab} - L) M = (L^M_{ba} - L) V + h(b-a) L (MV) + O(h^2)$$

where for example $L^V_{ab} f(x) = \sum_y W(x,y) \exp[h(bV(y) - aV(x))] [f(y) - f(x)]$. The symmetry in (23) then easily follows from averaging the identity (24). We add however a different proof that connects with the response formula (12).

**Proof of Proposition 2.** For observables $Q$ which are of the form $Q = LM$, the linear response is given by (12).

$$R^\rho_{LM,V}(t,s) = \frac{\partial}{\partial s} [a\langle V(x_s) L M(x_t) \rangle_\rho + b\langle V(x_s) M(x_t) \rangle_\rho]$$

When we consider a constant perturbation $h_s = h$, we get the integrated form of the response function:

$$R(t) = \int_0^t ds R^\rho_{LM,V}(t,s)$$

$$= a\langle [V(x_t) - V(x_0)] L M(x_t) \rangle_\rho + b\langle [L V(x_t) - L V(x_0)] M(x_t) \rangle_\rho$$

It suffices to take $t \to \infty$ to see the appearance of (23). The exchange of the limits $h \to 0$ and $t \uparrow +\infty$ is trivial in the case considered, so that for constant $h_t = h$

$$\lim_t R(t) = \chi_{MV}^{ab}$$

$\square$
7. Response and dynamical fluctuations

We turn to the interpretation of the response functions in terms of fluctuation theory. The standard interpretation of the equilibrium response \([4]\) is in terms of energy dissipation, and that is why \([5]\) is called the fluctuation-dissipation theorem even though it really deals with response. That terminology and corresponding interpretation remains true and useful for the first term in \([20]\) at least when considering the flux in excess to what already was present (since we now deal with nonequilibrium). That was explained in \([2]\), section 5, and we also see it in the identity \([18]\) which can be interpreted as a conservation of energy. From a probabilistic point of view it is more interesting to concentrate on what is new with respect to equilibrium, the second term in \([20]\).

The way of responding and the way of fluctuating are like each other’s time-reversals. For inspiration, we turn again to the equilibrium (hence, time-reversible) case, where the response to a perturbation typically goes along the same path as that of a spontaneous fluctuation; that is sometimes called Onsager’s regression hypothesis and in our context it could be summarized as \(L = L^*\) where \(L^*\) is the adjoint in the \(\rho\)-scalar product. In nonequilibrium the regression of a fluctuation is also the time-reversal of its appearance, but now the time-reversal is not trivial. In particular the second term in \([20]\) is

\[
- b \sum_x \rho(x) V(x) L^* e^{(t-s)L} Q(x)
\]

which now cannot be written as a time-derivative as in the first term of \([20]\). Yet, it is related to a fluctuation, as we explain now.

Suppose a (constant) perturbation \(V\) is added to the system. The system responds but in the long time, the perturbation also installs a new stationary law. Let us denote this new stationary law by \(\mu\). On the other hand one can compute the probability that in the unperturbed dynamics \(\mu\) occurs as a fluctuation. This takes us to the dynamical fluctuation theory for Markov processes, started by \([5]\), see also e.g. in \([3]\). Without going to the full details it suffices here to recall that for an ergodic Markov process with backward generator \(L\) there is a fluctuation functional \(I(\mu)\) on the probability laws \(\mu\) on \(K\), of the form

\[
I(\mu) = - \inf_{g > 0} \sum_x \mu(x) \frac{Lg}{g}(x)
\]

(26)

for which in the sense of the theory of large deviations

\[
\text{Prob}_\rho[p_\tau \simeq \mu] \simeq e^{-\tau I(\mu)}, \quad \tau \uparrow +\infty
\]
for the empirical distribution
\[ p_\tau(x) = \frac{1}{\tau} \int_0^\tau \delta_{x_t,x} \, dt, \quad \text{with } \delta_{a,b} = 0 \text{ if } a \neq b \text{ and } \delta_{a,b} = 1 \text{ if } a = b \]
of occupation times over the time-interval \([0, \tau]\). We refer to [9] for a dynamical fluctuation theory in the context of the present paper. In a sense, \(\exp -\tau I(\mu)\) gives the plausibility of the long-term (= \(\tau\)) appearance of (= dynamical fluctuation to) the statistics \(\mu\). Taking \(g = \exp(bhM/2)\) in (26), we see
\[ I(\mu) = -\inf_M \left\{ \sum_x \mu(x) \left[ \sum_y W(x,y)e^{\frac{bh}{2}[M(y)-M(x)]} - \sum_y W(x,y) \right] \right\} \quad (27) \]
That \(M\) can now be interpreted as a potential. The infimum in (27) gets reached at \(M = V\), the potential for which \(\mu\) is the stationary law. Already here we see a complementarity between response and fluctuations: a perturbation \(V\) gives a new stationary law \(\mu\), and to find the probability of a fluctuation \(\mu\) in the original dynamics, one has to find exactly this \(V\). But there is also a quantitative relation, in particular as realized in the second term in (20), as we prove in the next proposition.

**Proposition 3.** The dynamical fluctuation functional \(I(\mu)\) satisfies
\[ I(\mu) = -\frac{bh}{4} \sum_x \mu(x) LV(x) + o(h^2) \quad (28) \]

**Proof of Proposition 3.** For our case we can exchange the limit by the infimum and the small \(h\) limit, see also [8]. We can then compute (26) to first order in \(h\) by taking \(M = bhV/2\) in (27), and expanding
\[ \sum_{x,y} \mu(x) W(x,y) \left[ 1 - e^{bh[V(y)-V(x)]/2} \right] = -\frac{bh}{2} \sum_{x,y} \mu(x) W(x,y)[V(y) - V(x)] \]
\[ -\frac{b^2h^2}{8} \sum_{x,y} \rho(x) W(x,y) (V(y) - V(x))^2 + o(h^2) \quad (29) \]
where we have used already that \(\langle LV \rangle_\rho = 0\) by stationarity. For the second term we can replace the \(\rho(x)\) by \(\mu(x)\) because we are already at second order in \(h\) and write
\[ -\frac{b^2h^2}{8} \sum_{x,y} \mu(x) W(x,y) (V(y) - V(x))^2 + o(h^2) = \]
\[ \frac{bh}{4} \sum_{x,y} \mu(x) W(x,y)[V(y) - V(x)] [1 - e^{bh[V(y)-V(x)]/2}] \]
\[ = \frac{bh}{4} \sum_{x,y} \mu(x) W(x,y)[V(y) - V(x)] \]
because $\mu$ is invariant under the perturbed dynamics. Collecting all terms we get the result (28).

Of course the $LV(x)$ in the response formulæ (12)–(20)–(23) has the usual meaning of being the expected rate of change in $V$ while at $x$. Proposition 3 adds the interpretation that it can also be seen as the change in escape rate from $x$ when adding a potential $V$. From (28) the second term in (20) gives a correlation with a generalized escape rate and thus relates with the dynamical fluctuations of the occupation times, [9, 8].

8. Conclusion

We have generalized the results of [1, 2] to the perturbation first considered by [4], Proposition 1. We have also added a stationary response relation and noted a new symmetry, Proposition 2. The fluctuation interpretation of [2] remains intact, Proposition 3.

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