The fluctuation-dissipation relation: how does one compare correlation functions and responses?

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Abstract. We discuss the well known Einstein and the Kubo fluctuation-dissipation relations (FDRs) in the wider framework of a generalized FDR for systems with a stationary probability distribution. A multivariate linear Langevin model, which includes dynamics with memory, is used as a treatable example to show how the usual relations are recovered only in particular cases. This study brings to the fore the ambiguities of a check of the FDR done without knowing the significant degrees of freedom and their coupling. An analogous scenario emerges in the dynamics of diluted shaken granular media. There, the correlation between position and velocity of particles, due to spatial inhomogeneities, induces violation of usual FDRs. The search for the appropriate correlation function which could restore the FDR can be more insightful than a definition of ‘non-equilibrium’ or ‘effective temperatures’.

Keywords: Brownian motion, granular matter, fluctuations (theory), stationary states
1. Introduction

The idea of a link between dissipation and fluctuations dates back to Einstein with his work on the Brownian motion [1] and his relation between mobility (which is a non-equilibrium quantity) and the diffusion coefficient (which is an equilibrium quantity). Later Onsager [2, 3], with the regression hypothesis, and Kubo [4, 5], with linear response theory, investigated in a deep way the issue of the fluctuation-dissipation relation (FDR). In the last few decades there has been renewed interest in this topic; see the contributions of Morris, Evans, Cohen, Gallavotti and Jarzynski [6]–[8] to cite just some of the most well known attempts (for a recent review, see [9]).

The FDR theory was originally introduced in the Hamiltonian systems near thermodynamic equilibrium. However, it is now clear that a generalized FDR exists, under very general assumptions, for a large class of systems with a ‘good statistical behavior’, i.e. with a relaxation to an invariant (smooth) probability distribution. We stress that such a condition is quite common, e.g. in any system with a finite number of degrees of freedom whose evolution rules include some randomness (for instance nonlinear Langevin equations). Unfortunately the explicit form of generalized FDR depends on the shape of the invariant probability distribution (which is typically unknown); however this is only a technical difficulty without conceptual consequences [9].

We are not concerned with systems without a stationary probability distribution, e.g. systems showing ageing [10, 11] and glassy behavior [12]. On the contrary, we consider here systems with an invariant probability distribution satisfying the hypothesis for the
validity of the generalized FDR mentioned before. For such systems, in our opinion, there is some confusion about what form of FDR has to be expected. When couplings between the chosen observable and other degrees of freedom are ignored, the wrong FDR is expected, i.e. the response function is compared to the wrong correlation: this leads to what is often called a ‘violation’ of FDR.

The structure of the paper is the following. At first, in section 2, we discuss the different kinds of FDR obtained in the statistical mechanics framework. In section 3 we analyze a one-dimensional Langevin equation with memory, which can be mapped to a multivariate Langevin equation without memory: this example can be worked out analytically and illustrates well all the main points of our discussion. In section 4 some numerical results on a driven granular gas model are discussed, to support our general discussion with physical examples. Section 5 is devoted to concluding remarks.

2. The linear response in statistical mechanics

Let us briefly recall three different kinds of fluctuation-dissipation relations (FDR), commonly used in statistical mechanics when a small impulsive perturbation is applied to a stationary system. These three formulae share the feature of relating the system’s linear response to an appropriate two-time correlation computed in the unperturbed system. Anyway, these relations have different fields of application and must be adapted with care. For a more pedagogical introduction, we first set the notation, and then we discuss the three FDR versions.

2.1. Linear response functions

We adopt the following notation: $\delta(t)$ denotes the Dirac delta function, and $\delta_{ij}$ the Kronecker delta; we use the overline $\overline{\cdot}$ for non-stationary averages over many realizations and $\langle \cdot \rangle$ for averages using the unperturbed stationary probability in phase space (assuming ergodicity, this is equivalent to a time average over a long trajectory). Accordingly, we use the shorthand notation

$$C_{AB}(t) = \langle A(t)B(0) \rangle$$

(1)

to denote the two-time correlation function, between observables $A(X(t))$ and $B(X(t))$, with $X(t)$ the state of the system at time $t$. Let us introduce the matrix of linear response functions, whose $ij$ element reads

$$R_{X_iX_j}(t) \equiv \frac{\delta X_i(t)}{\delta X_j(0)},$$

(2)

i.e. the mean response of the variable $X_i$ at time $t$ to an impulsive perturbation applied to a variable $X_j$ at time 0. If the dynamics of the system is given, for instance in the form $dX(t)/dt = f(X)$, the mean linear response of the $i$th degree of freedom to a small perturbation of the $j$th component of the vector field $f_j \rightarrow f_j + \delta f_j$ can be expressed as

$$\overline{\delta X_i(t)} = \int_{-\infty}^{t} ds \, R_{X_iX_j}(t - s) \delta f_j(s).$$

(3)

The case of an impulsive perturbation at time 0, $\delta f_j = \delta X_j(0)\delta(t)$, gives back the definition (2).
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Let us also consider the historically important case of a Hamiltonian system at thermal equilibrium: in this case the perturbation is typically defined on the Hamiltonian, i.e. $H \to H + \delta H$, with $\delta H \equiv -\delta h(t)B(X)$. A linear response function of an observable $A$ to an impulsive field $\delta h(0)\delta(t)$ at time $t = 0$, $R_{Ah}(t) = \delta A(t)/\delta h(0)$ determines the behavior of $\delta A(t)$ for a generic small perturbation $\delta h(t)$:

$$\delta A(t) = \int_{-\infty}^{t} ds \, R_{Ah}(t-s)\delta h(s).$$

(4)

There are no conceptual differences between the two procedures for perturbing the state (i.e. with a $\delta X_i(0)$ or the introduction of an extra term in the Hamiltonian): we can simply consider $A$ and $B$ as two variables of the system. For instance, consider the case where $X$ is the position of a colloidal particle evolving according to

$$\dot{X}_i = -\frac{1}{\gamma} \frac{\partial H}{\partial X_i} + \sqrt{\frac{2T}{\gamma}} \eta_i,$$

(5)

with $\eta_i$ independent normalized white noises, i.e. Gaussian processes with $\langle \eta_i \rangle = 0$ and $\langle \eta_i(t)\eta_j(t') \rangle = \delta_{ij}\delta(t-t')$. Here, the effect of a perturbation $\Delta H = -X_j \delta h(t)$ is equivalent to a $\delta f_i = \delta_{ij}(\delta h(t)/\gamma)$ and therefore, from a comparison of equations (3) and (4), one has $R_{Xih} = R_{X,i}/\gamma$.

2.2. Three different fluctuation-dissipation relations

We can now discuss the three forms of FDR that we are interested in:

(i) The generalized FDR, denoted as GFR in the following,

$$R_{X_iX_j}(t) = C_{X_iS_j}(t),$$

(6)

where $S_j$ (see below) depends on the invariant distribution density in phase space. This relation is valid (under quite general assumptions; see [13]–[17], [9]) in a dynamical system whose state is completely determined by the phase space coordinate $X$, and whose dynamics induces an invariant measure of phase space $\rho(X)$,

$$S_j = -\frac{\partial \log \rho(X)}{\partial X_j},$$

(7)

so the correlation reads

$$C_{X_iS_j}(t) = -\left\langle X_i(t)\frac{\partial \log \rho(X)}{\partial X_j} \right\rangle.$$

(8)

(ii) The so-called Einstein relation, in the following referred to as EFR$^5$,

$$R_{AA}(t) \equiv \frac{\delta A(t)}{\delta A(0)} = \frac{C_{AA}(t)}{C_{AA}(0)}.$$

(9)

$^4$ More precisely one assumes that $\rho(X)$ is a smooth non-vanishing function. This condition certainly holds if some noise is included in the dynamics.

$^5$ For simplicity we adopt the name ‘Einstein relation’ which, in the literature, has been typically used to denote the time integral of relation (9), e.g. the formula $\mu = \beta D$ relating the mobility $\mu$ to the self-diffusion coefficient $D$. 

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The most well known example of the above relation is given by a Brownian colloidal particle diffusing in an equilibrium fluid at temperature $T$. Such a system is described by a linear Langevin equation

$$m \ddot{v} = -\gamma v + \sqrt{2\gamma T} \eta,$$

where $\eta$ is a normalized white noise, i.e. a Gaussian process with $\langle \eta \rangle = 0$ and $\langle \eta(t)\eta(t') \rangle = \delta(t - t')$. It is easy to show that after a small impulsive force $\delta h(0) \delta(t)$ at time 0, the velocity perturbation, which at $t = 0$ is $\delta v(0) = \delta h(0)/m$, decays as $\delta v(t) = \delta v(0)e^{-\gamma t}$. On the other hand, since $C_{vv}(t) = C_{vv}(0)e^{-\gamma t}$, where $C_{vv}(0) = \langle v^2 \rangle = T/m$, the EFR (9) holds, with $A \equiv v$ (see [18]). The Green–Kubo relations, relating transport coefficients to the time integral of unperturbed current–current correlations, are the extension of relation (9) to generic transport processes.

(iii) The classical Kubo relation, hereafter denoted as the KFR,

$$R_{Ah} = -\beta \frac{d}{dt} C_{AB}(t). \quad (11)$$

This relation holds—for instance—when a Hamiltonian system, whose statistics is described by the canonical ensemble with temperature $T = 1/\beta$, is perturbed by a Hamiltonian variation $\delta \mathcal{H} = -\delta h(t) B$, which defines the perturbing force $h$ and the corresponding conjugate field $B$ (see [5,9]). Relation (11) also holds for Langevin equations with a gradient structure, e.g. equation (5). Introducing the quantity $\chi_{AB}(t) = \int_0^t R_{Ah}(t') dt'$, from (11) one has

$$\chi_{AB}(t) = \beta C_{AB}(0) - \beta C_{AB}(t). \quad (12)$$

In some of the literature [19]–[21] a deviation from (12) is indicated as a failure of FDR, a mark of being far from equilibrium, and is used to define new ‘non-equilibrium’ temperatures.

As the name suggests, the GFR (iii) includes both EFR (i) and KFR (ii) for some choices of the dynamics or of the stationary distribution $\rho(X)$ [9]. This can be shown for the case $A = X_i$ and $B = X_j$ and is easily generalized to any other case, as discussed above:

- **GFR → EFR:** this happens when the invariant distribution in phase space is of the form $\rho(X) = \exp(-1/2T) \sum_i X_i^2)/Z$ (Z being a normalizing constant); then one has $S_j = X_j/T$ and one immediately obtains EFR starting from relation GFR.

- **GFR → KFR:** this happens for Hamiltonian systems in the canonical ensemble, or Langevin equations with gradient structure when a small force is applied; in both cases one has $\rho(X) = \exp[-\beta \mathcal{H}(X)]/Z$, so the GFR involves the quantity $S_j = \beta(\partial \mathcal{H}/\partial X_j)$. If the dynamics is given, for instance, by an overdamped Langevin equation of the kind (5), one has that $S_j = -\beta \gamma X_j$, i.e. $R_{X_i, X_j} = \beta \gamma \langle X_i(t)X_j(0) \rangle$ and, considering the discussion after equation (5), the KFR $R_{X_i, h} = \beta \langle X_i(t)X_j(0) \rangle$ is immediately derived.

For this last quantity we use notation where the second subscript $B$ directly refers to the observable conjugate to the perturbed field $h$: even if it is not self-evident, this has the advantage of being coherent with the notation widely used in the literature.
3. The Langevin equation with memory

Let us now consider a system that does not necessarily fall either under the hypotheses of EFR or under those of KFR. Our choice here is a linear stochastic equation with memory:

\[ m\dddot{x} = -kx - \int_{-\infty}^{t} \Gamma(t-t')\dot{x}(t') \, dt' + \eta(t), \]  

(13)

where \( m \) is the mass of the tracer, \( k \) is the constant of an elastic force, \( \Gamma(t-t') \) is the friction kernel, \( \eta(t) \) is a stochastic force acting as a thermostat.

When there is no memory, i.e. \( \Gamma(t-t') = 2\gamma\delta(t-t') \) and \( \langle \eta(t)\eta(t') \rangle = 2\gamma T\delta(t-t') \), the usual Langevin equation is recovered, leading to EFR in the case \( k = 0 \), equation (10), or KFR in the overdamped case, equation (5).

For a generic memory kernel, Kubo [5] has also shown that EFR or KFR are recovered, provided that \( \langle \eta(t)\eta(t') \rangle = T\Gamma(t-t') \).

(14)

Here we consider a memory kernel of the kind

\[ \Gamma(t-t) = 2\gamma_l\delta(t-t') + \gamma_s t \exp \left( \frac{t-t'}{\tau_s} \right), \]

(15)

and a noise \( \eta(t) = \rho_l(t) + \rho_s(t) \) where \( \rho_l(t) \) and \( \rho_s(t) \) are two independent Gaussian processes with zero means and

\[ \langle \rho_l(t)\rho_l(t') \rangle = 2\gamma_l T\delta(t-t'), \quad \langle \rho_s(t)\rho_s(t') \rangle = T_s \frac{\gamma_s}{\tau_s} e^{-|t-t'|/\tau_s}, \]

(16)

so condition (14) is recovered when \( T_l = T_s \equiv T \) (the ‘s’ and ‘l’ subscripts stand for ‘slow’ and ‘fast’ respectively). In general, however, \( T_l \neq T_s \). Note also that \( T_l \) and \( T_s \) have the dimension of a temperature: indeed the model in its overdamped limit has been proposed as an example of a system coupled to two different baths acting on different timescales [19,20].

3.1. A Markovian equivalent model

The first observation about the system under study is that, because of the memory term, its dynamics after time \( t \) cannot be deduced from the knowledge of \( x \) and \( v \) at time \( t \): in fact, the evolution depends on its history, i.e. the dynamics is non-Markovian, and the GFR cannot be directly applied.

However, it is possible to recover Markovianity, at the price of adding additional degrees of freedom. In other words, it is possible (and this will be done in section 3.2) to recast equation (13) as a linear, multi-dimensional, Langevin equation:

\[ \frac{dx}{dt} = -Ax + \phi, \]

(17)

where \( x \) and \( \phi \) are \( N \)-dimensional vectors and \( A \) is a real \( N \times N \) matrix, in general not symmetric. In addition, now \( \phi(t) \) is a Gaussian process, with covariance matrix

\[ \langle \phi_i(t')\phi_j(t) \rangle = \delta(t-t')D_{ij}, \]

(18)
and the real parts of $A$’s eigenvalues are positive. The stationary probability density is [22]

$$P(x) = (2\pi)^{-N/2} |\text{Det} \sigma|^{-1/2} \exp \left\{ -\frac{1}{2} \sum_{ij} \sigma^{-1}_{ij} x_i x_j \right\},$$  \hspace{1cm} (19)$$

where $\sigma$ is a symmetric matrix determined by the following relation:

$$D = A \sigma + \sigma A^T.$$ \hspace{1cm} (20)

We can now explicitly study the fluctuation and response properties of the system since the dynamics, being now Markovian, satisfies the hypothesis of applicability of GFR. First, we recall the definition of the correlation matrix $C_{ij}(t) = \langle x_i(t) x_j(0) \rangle$, in the stationary state, which is time-translationally invariant. Then, using the equation of motion, it is immediately verified that $\dot{C}(t) = -AC(t)$, with the initial condition given by the covariance matrix, between degrees of freedom at equal time: $C(0) = \sigma$. The corresponding solution is

$$C(t) = \exp(-At)\sigma.$$ \hspace{1cm} (21)

Note that, in general, $\sigma$ and $A$ do not commute. It is also straightforward to recover the response function $R(t) = \exp(-At)$, since the GFR imposes the following equation:

$$R(t) = C(t)\sigma^{-1}.$$ \hspace{1cm} (22)

In general this function can be written as

$$\sum_{\alpha} R_{\alpha} \exp(-\lambda_\alpha t),$$ \hspace{1cm} (23)

where $R_{\alpha}$ are constant matrices, and $\lambda_\alpha$ are the eigenvalues of $A$. The $i, j$ element of the matrix $R(t)$ is the response function $R_{X_i, X_j}(t)$ for the corresponding degrees of freedom. However, at odds with EFR and KFR cases, this quantity cannot be expressed in terms of the correlation $C_{X_i, X_j}(t)$ only, since in general all the degrees of freedom are coupled:

$$R_{X_i, X_j}(t) = \sum_k (\sigma^{-1})_{kj} C_{X_k, X_k}(t),$$ \hspace{1cm} (24)

which appears as a violation of EFR or KFR, even if GFR is still valid.

In the following, we will explicitly walk through this analysis in two different limit conditions:

(i) the free case, when the harmonic force $kx$ can be neglected;

(ii) the overdamped case, when inertia $m\ddot{x}$ can be neglected.

### 3.2. Dynamics of the free particle

In the limit $k = 0$, and setting $m = 1$ without loss of generality, equation (13) becomes

$$\dot{v} = -\gamma v - \frac{\gamma_s}{\tau_s} \int_{-\infty}^{t} \frac{v(t')}{\tau_s} e^{-(t-t')/\tau_s} v(t') \, dt' + \rho_I(t) + \rho_s(t),$$ \hspace{1cm} (25)$$

where we have introduced velocity $v \equiv dx/dt$. 

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Equation (25) can be mapped to (17) by
\[
\begin{pmatrix}
\dot{v} \\
\dot{u}
\end{pmatrix} = -\begin{pmatrix}
\frac{\gamma_f}{\tau_s} & \frac{\gamma_s}{\tau_s} \\
-\frac{1}{\tau_s} & \frac{1}{\tau_s}
\end{pmatrix} \begin{pmatrix}
v \\
u
\end{pmatrix} + \begin{pmatrix}
\sqrt{\frac{2\gamma_f}{\tau_s}} \phi_1(t) \\
\sqrt{\frac{2\gamma_s}{\tau_s}} \phi_2(t)
\end{pmatrix},
\]
where \(\phi_1(t)\) and \(\phi_2(t)\) are independent normalized white noises, and \(u(t)\) is an auxiliary variable:
\[
u(t) = \frac{1}{\tau_s} \int_{-\infty}^{t} e^{-(t-t')/\tau_s} \left( v(t') + \sqrt{\frac{2T_s}{\gamma_s}} \phi_2(t') \right) dt'.
\]

Defining \(\alpha = \gamma_f/\gamma_s, \nu = \tau_s \gamma_s, \zeta^{-1} = (1+\alpha)(1+\nu \alpha)\) and \(\Delta T = T_s - T_1\), a straightforward calculation of the covariance matrix gives
\[
\sigma = \begin{pmatrix}
T_f + \zeta \Delta T & -\alpha \zeta \Delta T \\
-\alpha \zeta \Delta T & T_s/\nu - \alpha \zeta \Delta T
\end{pmatrix}.
\]

The more general formula for the response as a function of correlations is given by the GFR, equation (6):
\[
\frac{\partial v(t)}{\partial v(0)} = \sigma_{11}^{-1} \langle v(t)v(0) \rangle + \sigma_{12}^{-1} \langle v(t)u(0) \rangle.
\]

We can observe two different scenarios: in the case \(T_f = T_s \equiv T\), i.e. \(\Delta T = 0\), \(\sigma\) is diagonal with \(\sigma_{11} = T\) and \(\sigma_{22} = T/\nu\), condition (14) is restored and, independently of the values of other parameters, a direct proportionality between \(C_{vv}\) and \(R_{vv}\) is obtained (EFR). This is not the only case for this to happen: e.g. for fixed \(\nu = \tau_s \gamma_s\), one has two possible limits:
\[
\sigma \approx \begin{pmatrix}
T_s & 0 \\
0 & T_s/\nu
\end{pmatrix} \quad \text{or} \quad \sigma \approx \begin{pmatrix}
T_f & 0 \\
0 & T_s/\nu
\end{pmatrix},
\]
respectively for \(\gamma_f \ll \gamma_s\), i.e. \(\alpha \rightarrow 0\), and \(\gamma_f \gg \gamma_s\), i.e. \(\alpha \rightarrow \infty\). More generally, when \(T_f \neq T_s\), the coupling term \(\sigma_{12}\) differs from zero and a ‘violation’ of EFR emerges between the coupling of different degrees of freedom.

The situation is clarified by figure 1, where EFR is violated and the GFR holds: response \(R_{vv}(t)\), when plotted against \(C_{vv}(t)\), shows a nonlinear and non-monotonic graph. Anyway a simple linear plot is restored when the response is plotted against the linear combination of correlations indicated by formula (29). In this case it is evident that the ‘violation’ cannot be interpreted by means of any effective temperature: on the contrary, it is a consequence of having ‘missed’ the coupling between variables \(v\) and \(u\), which gives an additive contribution to the response of \(v\).

It is interesting to note that, even when \(T_f = T_s\) (i.e. \(\sigma_{12} = \sigma_{21} = 0\)), \(C_{vv}(t) \propto R_{vv}(t)\) is a linear combination of two different exponentials (see equation (23)); then its derivative is in general not proportional to \(R_{vv}\), i.e. the KFR does not hold. An example of this situation will be discussed in section 4 and figure 8.

The above consideration can be easily generalized to the case where several slow thermostats are present: let us suppose that there are \(N - 1\) thermostats at temperature \(T\) (the fast one and \(N - 2\) slow ones) and one at temperature \(T_1\). In this case it is possible to show that the off-diagonal terms in \(\sigma\) are proportional to \((T - T_1)\).
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Figure 1. Free particle with viscosity and memory, whose dynamics is given by equation (25): here we show the parametric plot of the velocity response to an impulsive perturbation at time 0, versus two different correlations. The Einstein relation, which is not satisfied, would correspond to a linear shape with slope 1 for the red dashed line. The black line shows that the GFR holds.

It is useful to stress the role of Markovianity, which is relevant for a correct prediction of the response. In fact the marginal probability distribution of velocity $P_m(v)$ can be computed straightforwardly from (25) and always has a Gaussian shape. From that, one could be tempted to conclude, inserting $P_m(v)$ inside GFR, that proportionality between response and correlation holds also if $T_f \neq T_s$, in contradiction with (28). This conclusion is wrong, as stated at the beginning of this section, because the process is Markovian only if both the variable $v$ and the ‘hidden’ variable $u$ are considered.

3.3. The overdamped limit with a harmonic potential

When $k \neq 0$, in the overdamped limit we can neglect the left-hand side term in (13), and the equation, after an integration by parts, reads

$$
\gamma_t \dot{x} = - \left( k + \frac{\gamma_s}{\tau_s} \right) x + \frac{\gamma_s}{\tau_s^2} \int_{-\infty}^{t} e^{-(t-t')/\tau_s} x(t') \, dt' + \rho_t(t) + \rho_s(t).
$$

(31)

This model has been discussed in the context of driven glassy systems [19, 20].

In order to restore Markovianity, we can map this equation as

$$
\begin{pmatrix}
\dot{x} \\
\dot{u}
\end{pmatrix} = - \begin{pmatrix}
k + \frac{\gamma_s}{\tau_s} & -\frac{\gamma_s}{\tau_s^2} \\
\frac{1}{\gamma_t} & \frac{1}{\tau_s}
\end{pmatrix} 
\begin{pmatrix}
x \\
u
\end{pmatrix} + \sqrt{\frac{2T_f}{\gamma_t}} \phi_1 + \sqrt{\frac{2T_s}{\gamma_s}} \phi_2,
$$

(32)
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Figure 2. Sketch of a simple model which is described by equation (32).

where, as before, $\phi_1$ and $\phi_2$ are independent white noises, while the auxiliary variable $u$ now reads

$$u(t) = \tau_s \int_{-\infty}^{t} e^{-(t-t')/\tau_s} \left( x(t') + \tau_s \sqrt{\frac{2T_s}{\gamma_s}} \phi_2(t') \right) dt'.$$

(33)

Equation (32) describes the overdamped dynamics of the model depicted in figure 2: a first particle at position $x$ is coupled to a thermostat with viscosity $\gamma_f$ and temperature $T_f$, and to the origin by a spring of elastic constant $k$; a second particle at position $u$ is coupled to a thermostat with viscosity $\gamma_s$ and temperature $T_s$; the coupling between the two particles is a spring of elastic constant $k' = \gamma_s/\tau_s$. The first particle, when uncoupled from the second particle, has a characteristic time $\tau_f = \gamma_f/k$.

Using non-dimensional parameters $\alpha = \gamma_f/\gamma_s$ and $\eta = \tau_s/\tau_f$, the covariance matrix $\sigma$ reads

$$\sigma = \begin{pmatrix} \frac{T_f}{k} + \frac{1}{\alpha} \frac{\Delta T}{k} & \frac{T_s}{k} - \frac{1}{\Gamma} \frac{\Delta T}{k} \\ \frac{T_s}{k} - \frac{1}{\Gamma} \frac{\Delta T}{k} & 1 + \frac{\Delta T}{k} \end{pmatrix},$$

(34)

where $\Gamma = 1 + (1/\alpha) + \eta$ and $\Delta T = T_s - T_f$. As we can see, a diagonal form for the matrix $\sigma$ is not recovered, even for $\Delta T = 0$, i.e. for this model the EFR never holds.

Let us consider now the KFR, with a force field $h$ coupled to the variable $x$. First, we note that, from (22),

$$\dot{C} = -RA\sigma$$

(35)

(where commutativity between $R$ and $A$ has been used). Therefore, in general, since $\delta x(t)/\delta h(0) = R_{xx}/\gamma_f$, one has

$$\frac{\delta x(t)}{\delta h(0)} = \frac{(A\sigma)^{-1}_{xx}}{\gamma_f} \dot{C}_{xx} - \frac{(A\sigma)^{-1}_{xu}}{\gamma_f} \dot{C}_{xu}.$$
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Figure 3. Overdamped motion of a particle with harmonic potential, viscosity and memory, whose dynamics is described by equation (32): we show here the parametric plot of integrated response versus two different self-correlations. The Kubo formula KFR, which is not satisfied, would correspond to a straight line of slope $-1$ for the blue dashed curve. The black line shows that the GFR holds.

Then, it is easy to see that the condition for having KFR is $(A\sigma)_{ux} = 0$. Here the matrix $A\sigma$ reads

$$A\sigma = \begin{pmatrix}
\frac{1}{\tau_f} & -\frac{1}{\tau_f} \\
\frac{1}{\tau_f} & \frac{1}{\tau_f} \\
\frac{1}{\tau_s} & \frac{1}{\tau_s} \\
\frac{1}{\tau_s} & \frac{1}{\tau_s} \\
\end{pmatrix},$$

(37)

and the condition $(A\sigma)_{ux} = 0$ is equivalent to $\Delta T = 0$.

As observed in figure 3, in analogy with the previous figure 1, the GFR always holds (solid lines), while the KFR is not verified because it ignores the coupling between relevant degrees of freedom. In general the local slope $s(t)$ of the parametric curve $\chi_{xx}(t)$ versus $C_{xx}(t)$ is given by

$$s(t) = -\frac{d\chi_{xx}}{dC_{xx}} = -\frac{d\chi(t)}{dt} \left[ \frac{dC_{xx}(t)}{dt} \right]^{-1},$$

(38)

which, for the model in equation (32), has two different limits:

$$1/s(t) \to T_f \quad \text{for } t \to 0,$$

(39)

$$1/s(t) \to 1/s_\infty = T_s - K\Delta T \quad \text{for } t \to \infty,$$

(40)

where

$$K = \frac{2 + \Gamma - \sqrt{\Gamma^2 - 4\eta}}{2\Gamma}.$$

(41)
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Actually, as observed in \[19,20\], when \(\tau_s \gg \tau_f\) the parametric plot \(\chi_{xx}(t)\) versus \(C_{xx}(t)\) takes the form of a broken line with two slopes: the point where the slope abruptly changes corresponds to the intermediate plateau of \(C_{xx}(t)\) (i.e. when \(\tau_s \gg t \gg \tau_f\)) and is located at a position on the \(\chi\)-axis, \(\sim y_0 \chi(\infty)\) with \(y_0 = (T_f/T_s)(k'/k)\): it becomes visible in the plot if \(y_0 \sim \frac{1}{2}\) (i.e. it is not close to 1 or 0). In this case, since \(K \to 0\), the two slopes are \(1/T_f\) and \(1/T_s\). This observation has driven a series of real and numerical experiments where the parametric plot \(\chi_{xx}(t)\) versus \(C_{xx}(t)\) (or their Fourier transforms for the frequency-dependent susceptibilities) were measured for some degree of freedom in slowly driven \[23\] or ageing \[24,25\] glassy systems, including models for densely packed granular materials \[26\]. In section 3.4 we discuss this limit and other interesting cases from the point of view of the GFR: this can be useful for understanding when the KFR-inspired parametric plot is meaningful and why.

### 3.4. Phenomenology of the \(\chi\) versus \(C\) parametric plot

In this section we probe the hypothesis that the relative relevance of the contributions \(((A\sigma)_{ax}/\gamma_f)\dot{C}_{ax}(t)\) and \(((A\sigma)_{ax}/\gamma_f)\dot{C}_{ax}(t)\) to the response \(\ddot{\delta}(t)/\ddot{\theta}(0)\) depends on the timescale of observation. In particular we consider the time integrals of these two contributions, such that \(\chi_{xx}(t) = Q_{xx}(t) + Q_{xx}(t)\); see equation (36):

\[
Q_{xx}(t) = \frac{(A\sigma)_{xx}^{-1}}{\gamma_f}\left[C_{xx}(0) - C_{xx}(t)\right],
\]

\[
Q_{xx}(t) = \frac{(A\sigma)_{xx}^{-1}}{\gamma_f}\left[C_{xx}(0) - C_{xx}(t)\right].
\]

The two eigenvalues of the matrix \(A\), determining the timescales of the system \(1/\lambda_+\) and \(1/\lambda_\), read

\[
\lambda_\pm = \frac{1}{2\tau_s}\left[\Gamma \pm \sqrt{\Gamma^2 - 4\eta}\right].
\]

As suggested by the interpretation given in figure 2, the parameters \(\tau_\pm = \gamma_f/k\) and \(\tau_s\) should act as timescales when they are separated enough. Indeed, an inspection of formula (44) shows that the inverses of \(\lambda_+\) and \(\lambda_-\) are proportional to \(\tau_\) and \(\tau_s\) when they are well separated, i.e. \(\tau_\gg \tau_\) or \(\tau_\gg \tau_s\). However this is a limit case, and more general conditions can be considered.

Our choices of parameters, always with \(T_\neq T_s\), are summarized in table 1: a case (a) where the timescales are mixed, and three cases (b), (c) and (d) where scales are well separated. In particular, in cases (c) and (d), the position of the intermediate plateau is shifted at one of the extremes of the parametric plot, i.e. only one range of timescales is visible. Of course we do not intend to exhaust all the possibilities of this rich model, but to offer a few examples which are interesting for the following question: what is the meaning of the usual ‘incomplete’ parametric plot \(\chi_{xx}\) versus \(C_{xx}\), which neglects the contribution of \(Q_{xx}\)?

The parametric plots, for the cases of table 1, are shown in figure 4. In figure 5, we present the corresponding contributions \(Q_{xx}(t)\) and \(Q_{xx}(t)\) as functions of time. We
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Figure 4. Parametric plots of integrated response $\chi_{xx}(t)$ versus self-correlation $C_{xx}(t)$ for the model in equation (32) with parameters given in table 1. Lines with slopes equal to $1/T_s$, $1/T_f$ and $s_\infty$ are also shown for reference.

Table 1. Table of parameters for the four cases presented in figures 4 and 5. The effective time of the ‘fast’ bath is defined as $\tau_f = \gamma_f/k$, while the effective spring constant coupling $x$ with $u$ is defined as $k' = \gamma_s/\tau_s$.

| Case | $T_s$ | $T_f$ | $\gamma_s$ | $\gamma_f$ | $\tau_s$ | $\tau_f$ | $k$ | $k'$ | $1/\lambda_-$ | $1/\lambda_+$ |
|------|-------|-------|------------|------------|----------|----------|-----|-----|--------------|--------------|
| a    | 5     | 0.2   | 20         | 40         | 30       | 20       | 2   | 2/3 | 47.3         | 12.7         |
| b    | 2     | 0.6   | 200        | 1          | 200      | 1        | 1   | 1   | 400          | 0.5          |
| c    | 2     | 0.6   | 100        | 100        | 2        | 1000     | 0.1 | 50  | 2000         | 1            |
| d    | 10    | 2     | 1          | 50         | 10       | 50       | 1   | 0.1 | 51.2         | 9.76         |

briefly discuss the four cases:

(a) If the timescales are not separated, the general form of the parametric plot (see figure 4(a)) is a curve. In fact, as shown in figure 5(a), the cross-term $Q_{xu}(t)$ is relevant at all the timescales. The slopes at the extremes of the parametric plot, which can be hard to measure in an experiment, are $1/T_f$ and $s_\infty \neq 1/T_s$. Apart from that, the main information of the parametric plot is pointing out the relevance of the coupling of $x$ with the ‘hidden’ variable $u$.

(b) In the ‘glassy’ limit $\tau_s \gg \tau_f$, with the constraint $y_0 = (T_f/T_s)(k'/k) \sim 1/2$, the well known broken line is found (see figure 4(b)), as discussed at the end of section 3.3. Figure 5(b) shows that $Q_{xu}(t)$ is negligible during the first transient, up to the first plateau of $\chi(t)$, while it becomes relevant during the second rise of $\chi(t)$ toward the final plateau.

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Figure 5. Integrated response $\chi_{xx}(t)$ as a function of time, for the model in equation (32) with parameters given in table 1. The curves $Q_{xx}(t)$ and $Q_{xu}(t)$, representing the two contributions to the response, i.e. $\chi_{xx}(t) = Q_{xx}(t) + Q_{xu}(t)$, are also shown. The violet curve with small circles represents the ratio $Q_{xu}(t)/Q_{xx}(t)$.

(c) If $\tau_f \gg \tau_s$, the parametric plot, figure 4(c), suggests an equilibrium-like behavior (similar to what one expects for $T_f = T_s$) with an effective temperature $1/s_\infty$ which is different from both $T_f$ and $T_s$. Indeed, this case is quite interesting: the term $Q_{xu}$ is of the same order of $Q_{xx}$ during all relevant timescales, but $Q_{xu}/Q_{xx}$ appears to be almost constant. This leads to observe a KFR-like plot with a non-trivial slope. The close similarity between $Q_{xx}$ and $Q_{xu}$ is due to the high value of the coupling constant $k' = \gamma_s/\tau_s$.

(d) In the last case, always with $\tau_f \gg \tau_s$, the contribution of $Q_{xu}(t)$ is negligible at all relevant timescales (see figure 5), giving rise to a straight parametric plot, shown in figure 4, with slope $1/T_f$. The low value of the coupling constant $k'$ is in agreement with this observation.

The lesson learnt from this brief study is that the shape of the parametric plot depends upon the timescales and the relative coupling $k'/k$. This is consistent with the fact that the correct formula for the response is always the GFR: $\delta x(t)/\delta h(0) = \dot{Q}_{xx} + \dot{Q}_{xu}$. However, the definition of an effective temperature through the relation $T_{eff}(t)(\delta x(t)/\delta h(0)) = \dot{Q}_{xx}(t)$ in general (see case (a)), does not seem really useful. In particular limits, the behavior of the additional term $Q_{xu}$ is such that $R \propto \dot{Q}_{xx}$ in a range of timescales, and therefore the measure of $T_{eff}$ becomes meaningful.
4. Granular gases

In the previous section we have shown for the analytically tractable case of linear Langevin equations how the presence of coupling among different degrees of freedom plays a role in the specific form of the GFR, which is in general different from the EFR and KFR. Such a feature is certainly not specific to the model considered: the non-equilibrium dynamics of a many-particle system may present the same kinds of non-trivial correlations among degrees of freedom, usually due to strong inhomogeneities generated by the lack of conservation laws valid at equilibrium. In these models the stationary distribution is not known and the use of the GFR for response analysis is rather subtle.

In the following we shall analyze granular gases in the steady state, which offer an interesting benchmark of this idea.

4.1. The model

Let us consider a $d$-dimensional model for driven granular gases [27]–[30]: $N$ identical disks (for $d = 2$) or rods (for $d = 1$) of diameter 1 in a volume $V = L \times L$ (for $d = 2$) or total length $L$ (for $d = 1$) with inelastic hard core interactions characterized by an instantaneous velocity change

$$v'_i = v_i - \frac{1+r}{2}[(v_i - v_j) \cdot \hat{n}]\hat{n},$$

(45)

where $i$ and $j$ are the labels of the colliding particles, $v$ and $v'$ are the velocities before and after the collision respectively, $\hat{n}$ is the unit vector joining the centers of particles and $r \in [0, 1]$ is the restitution coefficient which is equal to 1 in the elastic case. Each particle $i$ is coupled to a ‘thermal bath’, such that its dynamics (between two successive collisions) obeys

$$\frac{dv_i}{dt} = -\frac{1}{\tau_b}v_i + \sqrt{\frac{2T_b}{\tau_b}}\eta_i(t),$$

(46)

where $\tau_b$ and $T_b$ are parameters of the ‘bath’ and $\eta_i(t)$ are independent normalized white noises. We restrict ourselves to the dilute or liquid-like regime, excluding more dense systems where the slowness of relaxation prevents clear measures and poses doubts about the stationarity of the regime and its ergodicity: in practice we consider packing fractions (fraction of occupied volume) $\psi = N/(4V)$ in the range 0.01–0.5. Two important observables of the system are the mean free time between collisions, $\tau_c$, and the so-called granular temperature $T_g = \langle |v|^2 \rangle / d$.

In this model is possible to recover two different regimes. When the thermostat is dominant, i.e. when $\alpha = \tau_c/\tau_b \gg 1$, grains thermalize, on average, with the bath before experiencing a collision and the inelastic effects are negligible. This is an ‘equilibrium-like’ regime, similar to the elastic case $r = 1$, where the granular gas is spatially homogeneous, the distribution of velocity is Maxwellian and $T_g = T_b$. In contrast, when $\tau_c < \tau_b$, non-equilibrium effects can emerge such as deviation from Maxwell–Boltzmann statistics, spatial inhomogeneities and $T_g < T_b$ [27]–[30]. This ‘granular regime’, easily reached when the packing fraction is increased or inelasticity is reduced, is characterized by correlations among different particles. This peculiarity is the key ingredient for a correct response analysis of these systems, as we shall see in the following.
4.2. Failure of the EFR for strong dissipation

An analysis of the FDR for the previous model has been performed in [31, 32] (for $d = 2$) and [33] (for $d = 1$), and discussed also in [9]. Similar results are also obtained for other models, such as the inelastic Maxwell model on a $d = 2$ lattice driven by a Gaussian thermostat and mean field granular gases [34, 35]. The protocol used in numerical experiments cited above is the following:

(i) The gas is prepared in a ‘thermal’ state, with random velocity components extracted from a Gaussian with zero average and given variance, and positions of the particles chosen uniformly random in the box, avoiding overlapping configurations.

(ii) The system is allowed to evolve until a statistically stationary state is reached, which is set as time $0$: we verify that the total kinetic energy fluctuates around an average value which does not depend on initial conditions.

(iii) A copy of the system is obtained, identical to the original but for one particle, whose $x$ (for instance) velocity component is incremented by a fixed amount $\delta v(0)$.

(iv) Both systems are allowed to evolve with the unperturbed dynamics. For the random thermostats, the same noise realization is used. The perturbed tracer has velocity $v'(t)$, while the unperturbed one has velocity $v(t)$, so $\delta v(t) = v'(t) - v(t)$.

(v) After a time $t_{\text{max}}$ large enough the memory of the configuration at time 0 to have been lost, a new copy is made by perturbing a new random particle and the new response is measured. This procedure is repeated until a sufficient collection of data is obtained.

(vi) Finally the autocorrelation function $C_{vv}(t) = \langle v(t)v(0) \rangle$ in the original system and the response $R_{vv}(t) \equiv (\delta v(t)/\delta v(0))$ are measured.

The main result of those studies can be summarized: in the dilute limit (where the packing fraction $\psi \to 0$) or in the elastic limit ($r \to 1$), or in the limit of efficient thermostat $\alpha \to \infty$ (which is usually implied by the dilute limit), the Einstein relation, equation (9), is recovered for the velocity of a tracer particle, i.e. $R_{vv}(t) = C_{vv}(t)/T_g$. In contrast, when these conditions fail one can observe strong deviations from EFR.

In addition, there are some remarkable points:

- Non-Gaussian velocity distributions can appear also in the dilute regime, but they seem to have a minor role in the violations of EFR [32].
- The same scenario holds for dimension $d = 1$, where the tracer is sub-diffusive, i.e. where $\langle |x(t) - x(0)|^2 \rangle \sim t^{1/2}$ which also implies a non-monotonic $C_{vv}(t)$ with a power law tail $C_{vv}(t) \sim -t^{-3/2}$ for large $t$ [33].
- When a mixture of two different kinds of grains (e.g. with different masses or different restitution coefficients) is considered [36], the two components bear different granular temperatures and this leads to separated FDR in the dilute limit, i.e. a tracer satisfies the EFR with its own temperature, making it very difficult to obtain a neutral thermometer based on FDR.

The violation of the EFR becomes more and more pronounced as the inelasticity increases (lower values of $r$); the importance of the bath is reduced (lower values of $\alpha$) or the packing fraction $\psi$ is increased, as shown in figure 6. In correspondence with such variations of
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![Parametric plots for checking the EFR, for d = 1 and 2 models of inelastic hard core gases with a thermal bath. Different choices of parameters r (the restitution coefficient), α = τ_c/τ_b and ψ (the packing fraction) are shown: note that one can change α with ψ or r fixed (changing τ_b), but—in general—changes in ψ or r determine also changes in α (because of changes in τ_c). In all plots, the dashed line marks the Einstein relation \( R_{vv}(t)/C_{vv}(0) \).](image)

parameters, the correlation between velocities of adjacent particles is also enhanced, a phenomenon which is ruled out in equilibrium fluids. This effect can be directly measured in many ways; a possibility is shown in figure 7. In conclusion, the general lesson is that there is a quite clear correspondence between violations of the EFR and the appearance of correlations among different degrees of freedom.

4.3. A correct prediction of the response

Let us begin with an example explaining how a blind comparison between autocorrelation and response can be misleading. Clearly the EFR is satisfied in the elastic (‘equilibrium’) case, i.e. \( R_{vv}(t) \propto C_{vv}(t) \), thanks to the fact that, in the invariant measure, there is a very weak coupling between the tracer velocity and other degrees of freedom. However, it is also interesting to note that the shape of \( C_{vv}(t) \) is far from being an exponential also in the elastic (‘equilibrium’) case, because of the presence of two characteristic times \( τ_\text{b} \) and \( τ_c \). This non-exponential shape of \( C_{vv}(t) \) leads to a failure of the KFR, equation (12), as is evident in the lower left plot of figure 8. It is also instructive to plot the same quantities for a strongly inelastic case (see the right plots of figure 8), where an almost linear relation

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Figure 7. Static (same time) particle–particle correlations for energy fluctuations, for the \(d=1\) inelastic hard rods gas. In the inelastic case (squares) the coefficient is higher when the dissipation gets stronger, i.e. for small \(\alpha\) (left) or high packing fraction (right). The coefficient in the elastic case is also shown, which is negligible for all the values of the parameters.

seems to be at work. A first rough explanation is the lower granular temperature which is responsible for a higher mean free time \(\tau_c\), implying that \(\tau_c\) and \(\tau_b\) are slightly closer to each other with respect to the elastic case, making the \(C_{vr}(t)\) similar to a single exponential.

This example shows how the only way to have a correct prediction of the response can reside in the use of the GFR, which is always valid. For a quantitative comparison between correlation functions and response, one needs some hypothesis on the stationary probability distribution, in particular about the kind of coupling between different phase space variables. We report the result of a simple assumption, partly inspired by an idea of Speck and Seifert [37], where correlation among variables is mediated by a fluctuating ‘hydrodynamic’ velocity field \(u(x)\), in such a way that the relevant part of the stationary probability distribution for the tracer reads, approximately,

\[
P_m(v,x,t) \sim \exp \left\{ -\frac{(v - u(x,t))^2}{2T_g} \right\},
\]

(47)

with \(u(x,t)\) a local velocity average, defined on a small cell of diameter \(L_{\text{box}}\) centered in the particle. This is motivated by the observation that, at high density or inelasticities, spatially structured velocity fluctuations appear in the system for some time, even in the presence of external noise [30,38]. The generalized FDR following from assumption (47) reads

\[
R_{vv}(t) = C_s(t) = \frac{1}{T_g} \langle v(t) \{ v(0) - u[x(0)] \} \rangle,
\]

(48)

and is nicely verified in figure 9. In other words, one has a correction to the ‘naive’ expectation \(R_{vv}(t) = \langle v(t)v(0) \rangle/T_g\), i.e. the extra term \(-\langle v(t)u[x(0)] \rangle\) originated by the presence of a ‘hydrodynamic’ velocity field. A recent experiment [39] shows the presence, in a rather clear way, of a similar extra term (with respect to the KFR) for a colloidal particle in a toroidal optical trap, in a non-equilibrium steady state.
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2D, $\phi=47\%$

Figure 8. Comparison of an elastic (left) and inelastic (right) gas of hard disks coupled to the thermal bath for $d = 2$: the response $R_{vv}$ (denoted as $R$ for simplicity), the susceptibility $\chi_{vv}(t) = \int_0^t R_{vv}(t') \, dt'$ and the normalized velocity autocorrelation $C(t) = C_{vv}(t)/C_{vv}(0)$ are plotted in several different ways. The top graphs show the validity or breakdown of the Einstein relation $R = C$ for the elastic or inelastic case respectively; the bottom graphs display the parametric plot $\chi_{vv}$ versus $C_{vv}$ which would follow the form $\chi_{vv} = 1 - C$ if the second form of FDR, equation (11), i.e. $R_{vv} = -\dot{C}_{vv}$, held.

We conclude this section by underlining the connections between the results obtained for granular gases and Langevin equations. In general, the behavior of the Langevin model and of the granular model show some differences, for example the case expressed in figure 4 (case (b)) has no counterpart in these models and the ‘effective temperature’ approach is meaningless, even when timescales are well separated. However the use of GFR shows how, in both examples, the response is given by a sum of different contributions, and in some special limits, the cross-correlation term can be neglected and a comparison between the response and the autocorrelation does make sense. This happens in the ‘equilibrium-like’ cases of the Langevin model (cf figure 4, cases (c) and (d)) and in the dilute regime of the granular gas, in which there is no coupling between the velocity of the tracer and the ‘hidden variable’ embodied by the local velocity average. In contrast, when this approximation is not correct, a response–autocorrelation plot shows strong deviations from linearity, but can be predicted by taking into account all the contributions in the computation of the response.
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Figure 9. Response and correlations of the velocity tracer in the \(d = 2\) gas of inelastic hard disks for a choice of parameters such that FDR type (i) (the Einstein relation, equation (9)) is strongly violated. The dashed green curves show that the conjecture \(R_{vv}(t) = C_s(t) = (1/T_g) \langle v(t) \{ v(0) - u[x(0)] \} \rangle \) is probed, where \(u(x)\) is the local velocity field measured by coarse-graining in boxes (centered with the tracer) of size \(L_{box}\).

5. Conclusions

In this paper we have reviewed different forms of the fluctuation-dissipation relation for steady states. The most general one is the GFR, equation (6), which requires the knowledge of the relevant degrees of freedom and their reciprocal couplings in the system. When this knowledge is not accessible, the study of the response to a perturbation of a certain variable, compared to the correlation of that variable in the unperturbed state, has no simple meaning, in general.

As an example, we study in detail two limits of a generalized Langevin equation with memory, for a particle which moves in a harmonic potential and is in contact with two thermostats at different temperatures. In the overdamped case, the response–correlation parametric plot may reveal a broken line shape, where the two slopes are given by the inverse temperatures of the baths: a necessary, but not sufficient, condition for this to happen is that timescales are well separated. In the general case, however, the plot can be more difficult to read, showing intermediate ‘effective temperatures’, as well as a more general nonlinear shape.

Nevertheless, the problem can be recast as a Markovian dynamics, by means of the introduction of additional degrees of freedom. The Markovian dynamics has a stationary distribution and satisfies a general relation (GFR) between the response and a specific correlation function, which is related to the stationary measure and takes into account the coupling between degrees of freedom. We show how this coupling is responsible for the ‘violation’ of the usual FDR.

An interesting case where correlations play a role in the ‘violation’ of FDR is the dynamics of a tracer particle in a driven granular gas. Here the response is not proportional, in general, to the unperturbed autocorrelation and an effective temperature...
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does not seem to be informative, even when the timescales are well separated. Nevertheless a GFR should always be valid, provided an appropriate description of the dynamics is given. Indeed, as already stressed by Onsager and Machlup in their seminal work on fluctuations and irreversible processes [40], a basic ingredient for a ‘good statistical’ description is Markovianity. We recall their important caveat: how do you know you have taken enough variables, for it to be Markovian? We have seen that, following this suggestion, it is possible to have deeper insight into the so-called ‘violations of FDR’ and in some cases (e.g. in figure 9), one can try to guess the correct correlation involved in the dynamics.

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