

The many faces of fluctuation-dissipation relations out of equilibrium

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Abstract In this paper we offer to the reader an essential review of the theory of Fluctuation-Dissipation Relations (FDR), from the first formulations due to Einstein and Onsager, to the recent developments in the framework of stochastic thermodynamics of non-equilibrium system. We focus on two general approaches, somehow complementary, where out-of-equilibrium contributions to the FDR are expressed in terms of different quantities, related either to the stationary distribution or to the transition rates of the system. In particular, we discuss applications of the FDR in the general field of causation and inference, and in the contexts of non-equilibrium systems, such as spin models, granular media and active matter.

1 Introduction

The Fluctuation-Dissipation Relation (FDR) is among the few pillars of non-equilibrium statistical mechanics. The reason of its great relevance is rather transparent: it allows to compute the statistical response of a system to small external perturbations in terms of correlations of the unperturbed dynamics. In other words, one can understand how the system reacts to an external disturbance just looking at the statistical features in the absence of any perturbation: in such a way it is possible to determine perturbed properties (response) in terms of unperturbed features (correlations).

The FDR has been widely investigated in the context of turbulence (and more generally statistical fluid mechanics): for instance it plays a key role for the closure problem in the Kraichnan's approach [1]. Moreover, there is a wide interest of the scientific community active in geophysical systems, in particular, for climate dynamics, where it is very important to understand the features of the system under perturbations (such as a volcanic eruption, or a change of CO₂ concentration) in terms of the knowledge based on time series. Another very relevant field where the FDR has been used and investigated is the general theory of stochastic thermodynamics, with particular focus

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on models for colloidal systems, granular media and active matter. Finally, FDRs play a central role in the study of the non-equilibrium dynamics of slow relaxing systems, such as Ising models or spin glasses.

Since response and dissipation are intimately related (this intuitive fact is made more formal later in this section), in this paper we use “Fluctuation-Response” and “Fluctuation-Dissipation” in an interchangeable way. Historically, one of the first examples of Fluctuation-Response relation is given by the formula expressing the fluctuations of energy in an equilibrium system at temperature T with a (constant volume) heat capacity C_V , that reads

$$\langle E^2 \rangle - \langle E \rangle^2 = k_B T^2 C_V. \quad (1)$$

On the left hand side of the formula one has the fluctuations in an unperturbed system, while on the right hand side there is a quantity representing a response (the heat capacity), and the factor of proportionality between the two is the temperature (k_B is the Boltzmann constant). Einstein derived an analogous formula connecting the diffusivity D to the mobility μ for a Brownian particle dispersed in a solvent fluid at thermodynamic equilibrium:

$$D = k_B T \mu, \quad (2)$$

where again the unperturbed fluctuations (diffusivity) are proportional to response (mobility) through a factor of proportionality represented by the bath temperature T .

The two previous examples are instances of the larger class of so-called “static” equilibrium FDR, as they do not involve time-dependent quantities. In the first half of the 20th century a series of experimental and theoretical works made longer and longer the list of such kind of relations, always tying in the same way spontaneous fluctuations, response and temperature [2, 3]. A noticeable example from this list is the expression given by Nyquist in 1938, relating the fluctuations of voltage in a conducting wire where no potential differences or currents are externally applied (the so-called Johnson noise) to the resistance of the conductor and the temperature. The resistance is the analogous of the mobility and of the heat capacity in the previous equations, i.e. it represents a response. In this case it is also particularly simple to appreciate the equivalence between response and dissipation.

A first step towards the generalisation to a time-dependent - or dynamic - relation is represented by the regression hypothesis made by Onsager in 1931 [4, 5], which states that - for small perturbations from equilibrium - the system returns to equilibrium at the same rate as a fluctuation does at equilibrium. This fact is already contained in the Einstein relation above. By recalling the general connection between diffusivity and the velocity autocorrelation, i.e. that

$$D = \int_0^\infty dt \langle v(t) v(0) \rangle, \quad (3)$$

we can transform Eq. (2) into

$$\langle v(t) v(0) \rangle = k_B T R_{vF}(t), \quad (4)$$

with the identification

$$\mu = \int_0^\infty dt R_{vF}(t). \quad (5)$$

In the r.h.s. of Eq. (5) we define the so-called response function, $R_{vF}(t)$, which connects the mean variation of the particle’s velocity at time t with a perturbation of the external force applied at time 0.

In order to discuss in full generality the FDR, we need to give a general definition of response function, which is the central object of linear response theory. We restrict the discussion to the linear perturbation of stationary states, i.e. states which are invariant under translations of time, so that time-dependent correlation functions and response functions only depend on differences of times. Generalisations to non-steady states are mentioned in Section 2.

The response function $R_{O\mathcal{F}}(t)$ of the observable $O(t)$ to a time-dependent perturbation of a parameter or degree of freedom $\delta\mathcal{F}(t)$ is implicitly defined in the following relation

$$\overline{\Delta O(t)} = \int_{-\infty}^t dt' R_{O\mathcal{F}}(t-t') \delta\mathcal{F}(t'), \quad (6)$$

where $\overline{\Delta O(t)} = \overline{O(t)} - \langle O(t) \rangle_0$ represents the average deviation, at time t , of the observable O with respect to its average value in the unperturbed stationary system. Here $\overline{f(t)}$ denotes an average of the observable f at time t over many realisations of the same perturbation, while $\langle f \rangle_0$ denotes the average of f in the stationary unperturbed

state, which is not time-dependent. It is clear that, taking an impulsive shape for the external perturbation, i.e. $\delta\mathcal{F}(t) = \Delta\mathcal{F}\delta(t)$ (with $\delta(t)$ the Dirac delta distribution), one has

$$\frac{\overline{\Delta\mathcal{O}(t)}|_{imp}}{\Delta\mathcal{F}} = R_{O\mathcal{F}}(t), \quad (7)$$

which is also an operational definition of the response function. Here we stress that $\Delta\mathcal{F}$ has the dimensions of a time-integral of $\mathcal{F}(t)$. When (for instance) the perturbation has the shape of a Heaviside unit step function, i.e. $\delta\mathcal{F}(t) = \delta\mathcal{F}_0\Theta(t)$, then

$$\frac{\overline{\Delta\mathcal{O}(t)}|_{step}}{\delta\mathcal{F}_0} = \int_0^t dt' R_{O\mathcal{F}}(t'). \quad (8)$$

If $O(t)$ is the tracer's velocity along one axis and $\mathcal{F}(t)$ is the external force applied from time 0 to time ∞ to the tracer (parallel to that axis), the final velocity reached by the tracer is exactly $\delta\mathcal{F}_0 \int_0^\infty dt' R_{vF}(t')$, which explains the connection with the identification made in Eq. (5).

The FDR for systems with Hamiltonian \mathcal{H} at equilibrium with a thermostat at temperature T – historically attributed to Callen and Welton and immediately after generalised by Kubo [6] – reads:

$$R_{O\mathcal{F}}(t) = \frac{1}{k_B T} \langle O(t) \dot{A}(0) \rangle_0 = -\frac{1}{k_B T} \langle \dot{O}(t) A(0) \rangle_0, \quad (9)$$

where A is the observable (or degree of freedom) which is coupled to $\mathcal{F}(t)$ in the Hamiltonian to produce the perturbation, i.e. $\mathcal{H}(t) = \mathcal{H}_0 - \mathcal{F}(t)A$. It is easy to verify that if O is the tracer's velocity and $\mathcal{F}(t)$ is an external force applied to its x coordinate, Eq. (9) becomes Eq. (4). In conclusion the “dynamical” Einstein relation is a particular case of equilibrium FDR. From Eq. (9) one may get several possible variants, which are useful in different physical situations. A large amount of remarkable results concern, for instance, the time-Fourier transform of Eq. (9), as well as the relation connecting currents/flows and transport coefficients in spatially extended systems (the so-called Green-Kubo relations, see below) [2, 3].

The equilibrium FDR is valid also in the framework of stochastic processes, when they describe the dynamics of system fluctuating around thermal equilibrium. The main difference with the case considered by Kubo is that a stochastic process typically describes small systems, far from the thermodynamic limit, but the system size is in fact irrelevant for the purpose of the validity of the FDR. In the case of large systems (without long-range correlations), however, the averages are easily taken by means of one or few experiments, while in a stochastic process where noise is large, one needs to average over many realisations. An illustrative example is the so-called Klein-Kramers model which describes the dynamics of simple particle systems at thermal equilibrium [7]. In one dimension its stochastic differential equations read:

$$\frac{dx(t)}{dt} = v(t) \quad (10a)$$

$$m \frac{dv(t)}{dt} = -\frac{dU(x)}{dx} - \gamma v(t) + \sqrt{2\gamma k_B T} \xi(t), \quad (10b)$$

where $\xi(t)$ is a white Gaussian noise with $\langle \xi(t) \rangle = 0$ and $\langle \xi(t) \xi(t') \rangle = \delta(t - t')$, γ is the viscous damping, $U(x)$ is an external potential. The model can be easily generalised to $N > 1$ interacting particles in any dimensions. In the absence of the external potential, Eq. (10) coincides with the original Langevin equation proposed a few years after the theories of Einstein [8] and Smoluchovski [9] to explain diffusion in Brownian motion [10]. Its steady probability distribution (achieved with the condition $\gamma > 0$ and confining potential) is given by $P(x, v) \propto e^{-\mathcal{H}(x, v)/(k_B T)}$ with $\mathcal{H}(x, v) = mv^2/2 + U(x)$. Linear response theory, when applied to the Klein-Kramers model in its stationary state, gives exactly the same result as Eq. (9) [11, 3]. The Klein-Kramers process is Markovian with respect to the variables (x, v) , a property which is a rough approximation for the dynamics of a tracer which interacts with other particles in a fluid. Typically it has to be generalised to take into account retarded (hydrodynamic) effects, by the introduction of linear memory terms, e.g. by writing a Generalized Langevin Equation (GLE) [2]:

$$m \frac{dv(t)}{dt} = - \int_{-\infty}^t dt' \Gamma(t - t') v(t') + \eta(t), \quad (11)$$

where $\Gamma(t)$ is a memory kernel representing retarded damping, and $\eta(t)$ is a stationary stochastic process with zero average $\langle \eta(t) \rangle = 0$. The noise time-correlation – to comply with the requirement of thermodynamic equilibrium (i.e. steady Gibbs distribution and detailed balance) – must satisfy the so-called FDR of the second kind:

$$\Gamma(t) = \frac{1}{k_B T} \langle \eta(t) \eta(0) \rangle. \quad (12)$$

It is clear that Eq. (12) has the same structure of Eq. (9) and this motivates the name of the relation. The Markovian case (damping with zero memory) is obtained when $\Gamma(t) = 2\gamma\delta(t)$ (recalling that $\int_0^t dt' 2\gamma\delta(t')v(t') = \gamma v(t)$). For a more detailed discussion of the significance of this condition and its connection to detailed balance, we invite to read Section 4.1 of [12].

This brief review paper is organised as follows. In Section 2 we introduce two different possible approaches to the FDR, which are based either on the knowledge of the stationary distribution or on the knowledge of the dynamical rules of the model. Then, in Section 3, we discuss several applications of the FDR, in particular in the field of non-equilibrium systems, such as granular media and active matter. Finally, in Section 4, some conclusions are drawn.

2 Two approaches to non-equilibrium FDR

The first examples of FDR date back to Einstein's work on Brownian motion (1905), and to Onsager's regression hypothesis (1930's). Since initially the FDR was obtained for Hamiltonian systems in thermodynamic equilibrium, somehow there is a certain confusion on its real validity. Here we summarise two different generalizations of FDR which both hold for a broad class of systems, including the non equilibrium cases [3].

2.1 An approach based upon the knowledge of the stationary distribution

Let us consider a system whose stationary probability density $P_{st}(\mathbf{x})$ is non-vanishing everywhere, and wonder about the time behavior of the mean response of the variable $x_n(t)$ at time t under a small impulsive perturbation $\delta\mathbf{x}(0)$. We can write

$$\overline{\delta x_n(t)} = \left\langle x_n(t) \right\rangle_p - \left\langle x_n(t) \right\rangle$$

where $\left\langle \right\rangle_p$ and $\left\langle \right\rangle$ denote the average for the perturbed and the unperturbed systems respectively. For a Markov system we can write

$$\left\langle x_n(t) \right\rangle_p = \int x_n P_p(\mathbf{y}) W(\mathbf{y} \rightarrow \mathbf{x}, t) d\mathbf{x} d\mathbf{y}, \quad \left\langle x_n(t) \right\rangle = \int x_n P_0(\mathbf{y}) W(\mathbf{y} \rightarrow \mathbf{x}, t) d\mathbf{x} d\mathbf{y},$$

where $W(\mathbf{y} \rightarrow \mathbf{x}, t)$ is the probability of a transition from \mathbf{y} at time 0 to \mathbf{x} at time t , $P_0(\mathbf{y}) = P_{st}(\mathbf{y})$ and $P_p(\mathbf{y})$ is the initial distribution of the perturbed system.

In the case of an impulsive perturbation, the perturbed probability satisfies $P_p(\mathbf{y}) = P_{st}(\mathbf{y} - \delta\mathbf{x}(0))$ which allow us to derive a compact expression for $\overline{\delta x_n}$ when the perturbation is small:

$$\overline{\delta x_n(t)} = - \sum_j \left\langle x_n(t) \frac{\partial \ln P_{st}[\mathbf{x}(0)]}{\partial x_j(0)} \delta x_j(0) \right\rangle, \quad (13)$$

where the average is performed in the unperturbed system. Let us note that the assumption of small perturbation is necessary only in the last step of the derivation of Eq. (13) therefore, such a result can be generalized to the case of non-infinitesimal $\delta\mathbf{x}(0)$ [13]. As by-product we have that it is possible to avoid the criticism of van Kampen according to which it is not possible to rely on an expansion for small perturbations, because chaos makes them

grow exponentially [14]. On the contrary, in the derivation of the above result [15], there are only assumptions about $\delta\mathbf{x}(t=0)$ and therefore chaos has no relevance.

We can say that formula (13) summarizes the main results of the linear theory, e.g. in Hamiltonian systems and stochastic processes: in addition one understands the existence of a link between response and a suitable correlation function even in non-equilibrium systems [3]. For instance in inviscid hydrodynamics with an ultraviolet cutoff, in spite of the non trivial dynamics, since the presence of quadratic invariant, and a Liouville theorem, one has a Gaussian statistics and therefore a FDR holds for each of the variables, i.e. self-response functions to infinitesimal perturbations coincide with the corresponding self-correlation functions. Let us note that although $P_{st}(\mathbf{x})$ is Gaussian the dynamics is non linear and it is not easy to compute the correlation functions.

Beyond the many conceptual advantages of eq. (13) there is an obvious practical limit: the difficulty to determine $P_{st}(\mathbf{x})$, which is known only in some specific cases. In the next subsection we will discuss an approach which does not need the knowledge of $P_{st}(\mathbf{x})$.

Let us open a brief parenthesis on chaotic deterministic dissipative systems: because of the phase space contraction one has that the invariant measure is singular, typically with a multifractal structure, and therefore, Eq. (13) cannot be applied. A quite natural temptation is to add a small amount of noise, so that a smoothing of the invariant probability density allows for the use of the FDR. At a first glance such an approach can appear unfair. On the contrary the idea of the beneficial role of the noise, which seems to date back to Kolmogorov, has strong bases: a small noisy term in the evolution equations has the role of selecting the natural measure: one can say that in the numerical experiments the round-off errors of the computer play a positive role. It is quite natural to expect that the behaviors of the purely deterministic chaotic system are very close to those obtained by adding a small amount of noise; such a conjecture is widely confirmed by numerical computations [16].

A similar approach was extended by Seifert and Speck, who established interesting connections of the FDR with observables in the framework of stochastic thermodynamics, such as entropy production and housekeeping heat [17, 18, 19] (see also the next Section).

2.2 An approach based upon the knowledge of the dynamical model

When the dynamics of the system under study is defined in terms of transition rates or Langevin equations, but the stationary probability density function is not known, a complementary approach with respect to the one discussed in the previous subsection can provide a FDR valid also out of equilibrium. These kinds of FDRs have been derived in several different contexts, following different mathematical schemes (see discussion below).

The general approach dates back to the 60's of the 20th century, when Furutsu and Novikov independently derived, under general conditions, a FDR [20, 21] which expresses the response function of a Gaussian process in terms of the equilibrium time-correlation between the observed variable and the Gaussian noise itself. Nowadays, a method based on similar ideas - sometimes termed Malliavin weight sampling [22] - has been extended to include field theories through the Martin-Siggia-Rose-Jansen-de Dominicis approach [23, 24, 25] and employed in the context of particle-based glassy systems to numerically calculate effective temperature and susceptibility [26, 27, 28]. This allows one to express the response function in terms of suitable correlation functions of the state variables. We mention here examples for non-equilibrium Langevin dynamics driven by a time-dependent force both in overdamped [18, 29, 30, 31, 32] and underdamped regimes [33], or even in the presence of a non-linear Stokes force [34]. The non-equilibrium terms appearing in the generalized FDR have been interpreted in several ways: some authors focused on the different roles of entropic and frenetic contributions (for a recent review, see [35]), outlining their different nature with respect to the symmetry under time-reversal transformation; other approaches have focused on the connection with entropy production and heat [36, 17, 37].

The class of generalized FDR so far mentioned is expressed in terms of the correlation between the observable O and a function of both the state variables and their time-derivatives. Without loss of generality, the starting point for these relations is of the form:

$$R_{Ox_j}(t, s) = \langle O(t) \mathcal{M}_j[\mathbf{x}(s), \dot{\mathbf{x}}(s)] \rangle, \quad (14)$$

where, as usual, the average in the r.h.s. of Eq. (14) is performed through the unperturbed measure. \mathcal{M}_j is a function uniquely determined by the dynamics of the system under consideration that depends both on \mathbf{x} and $\dot{\mathbf{x}}$. Its functional form can be expressed in terms of known observables: for instance, in the case of continuous first order

dynamics of the kind

$$\dot{x}_j = f_j(\mathbf{x}) + \sqrt{2D_j}\eta_j, \quad (15)$$

where η_j is a white noise with zero average and unit variance, one has

$$\mathcal{M}_j = \frac{1}{2D_j}(\dot{x}_j - f_j). \quad (16)$$

The above result is general, holding in stationary or transient non-equilibrium regimes. In some cases, i.e. when the quantity \mathcal{M}_j can be measured, Eq. (14) may represent an advantage with respect to Eq. (13) (which depends upon the knowledge of the steady-state probability).

The explicit dependence on the time-derivative of the state variables, $\dot{\mathbf{x}}$, in Eq. (14) may still represent a source of complications. Restricting to the calculation of the response matrix, $R_{x_i x_j}(t)$, i.e. such that $O = x_i$, from Eq. (14) one can derive [38] a simpler expression for processes with additive Gaussian noises in the stationary state (the result can be easily generalized to the case of non-diagonal diffusion, not reported for conciseness):

$$R_{x_i x_j}(t) = -\frac{1}{2D_j} [\langle x_i(t) f_j(0) \rangle + \langle f_i(t) x_j(0) \rangle]. \quad (17)$$

Each element of the response matrix is given by the sum of two correlations: i) the temporal correlation between the observed variable and the force ruling the dynamics of the perturbed variable and ii) the temporal correlation between the force of the observed variable and the perturbed variable (that for the diagonal elements, $R_{x_i x_i}(t)$, is the same correlation of i) with swapped times). The two terms are equal only at equilibrium. On the contrary they differ when detailed balance does not hold. Note that the generalized FDR (17), differently from the forms (13) or (14), is not determined by the time-correlation between the observed variable evaluated at t and another observable at $s < t$. Moreover, path-integral FDRs require the explicit knowledge of the microscopic dynamics, at variance with the approach (13) which only requires a model of the stationary probability in phase space: it must be noticed that in experimental situations it can be simpler to formulate a model for the steady state probability rather than for the full dynamics. In both cases, however, one needs to individuate the relevant variables, an often underestimated aspect [39].

The generalized FDR (17) is particularly fascinating because the diagonal elements of the response matrix (r.h.s of Eq. (17)) are expressed in terms of the time-symmetric part of the anticipated/retarded equipartition relations while the non-diagonal elements represent the time-symmetric part of the anticipated/retarded Virial equation [38]. Indeed, because of the causality condition, we have $R_{x_i x_j}(t = 0) = \delta_{ij}$, so that the initial time elements of the response matrix contain the same information as the generalized equipartition and Virial equations holding out of equilibrium, namely:

$$D_i = \langle x_i f_i \rangle, \quad \langle x_i f_j \rangle = -\langle x_j f_i \rangle. \quad (18)$$

This physical interpretation has been discussed in detail in [38] and exploited in well-known examples, such as passive and active colloids both in underdamped and overdamped regimes, see also Section 3.4.

Let us also comment on the interesting case of discrete variables, relevant for instance for the Ising model or spin glasses, which requires some care. In particular, for spins $\sigma_i = \pm 1$, with $i = 1, \dots, N$, evolving according to a Master Equation with unperturbed transition rates from the configuration σ to the configuration σ' , $w(\sigma \rightarrow \sigma')$, in contact with a reservoir at temperature T , the response of an observable $O(\sigma)$ at a magnetic field \mathcal{F} switched on at time s on site j takes the following form [40]

$$R_{O\mathcal{F}}(t, s) = \frac{1}{2T} \left\{ \frac{\partial}{\partial s} \langle O(t) \sigma_j(s) \rangle - \langle O(t) B_j(s) \rangle \right\}, \quad (19)$$

where the quantity $B_j[\sigma]$ is defined by

$$B_j[\sigma(s)] = \sum_{\sigma'} [\sigma'_j - \sigma_j(s)] w[\sigma(s) \rightarrow \sigma']. \quad (20)$$

The equilibrium FDT (9) is obtained exploiting the property

$$\left\langle O(t) \sum_{\sigma'} [\sigma'_j - \sigma_j(s)] w[\sigma(s) \rightarrow \sigma'] \right\rangle_{eq} = -\frac{\partial}{\partial s} \langle O(t) \sigma_j(s) \rangle_{eq}, \quad (21)$$

valid when the average is taken at equilibrium [40, 41].

3 Applications

In this Section we discuss recent applications of the generalised formulae discussed above to different problems. We start with two more theoretical cases, namely the broad class of spin and disordered systems and the search for causality measurements, and we conclude with applications to paradigmatic macroscopic physical systems, that are granular and active systems, where the dynamics of each particle is intrinsically out of equilibrium.

3.1 The interesting case of causation through response

Among the many practical applications of the generalized FDR (13), its use in the field of causal inference has a particular conceptual interest. It is well known that, in order to understand the cause-effect relations holding between different elements of a system, measuring the degree of correlation of the variables may be, in general, of little help: two elements can be highly correlated even in the absence of a causal link, as summarized by the notorious adage “correlation does not imply causation”. The right way to characterize causal relations is indeed to *probe* the system under study, i.e. to perturb it in some way and to observe the effects of this external action, comparing them to the usual behavior of the system in the absence of perturbation [42, 43]; this is, for instance, the fundamental idea at the basis of Pearls’ formalism of counterfactual inference [44]. When dealing with physical systems, as discussed in the Introduction, the effect of an external perturbation is quantified by response functions, which are therefore natural indicators of causal relations [43, 45]. In this respect, a surprising consequence of Eq. (13) is that these observables can be estimated by measuring proper correlation functions in an *unperturbed* dynamics: in other words, the generalized FDR allows to infer causal relations without operating any external action on the system, i.e. without actually probing it.

To show the above point, let us consider the example of a linear stochastic dynamics for the three-dimensional vector (x_t, y_t, z_t) in discrete time, ruled by the following Markov process:

$$x_{t+1} = ax_t + \varepsilon y_t + b\eta_t^{(x)} \quad (22a)$$

$$y_{t+1} = ax_t + ay_t + b\eta_t^{(y)} \quad (22b)$$

$$z_{t+1} = ax_t + az_t + b\eta_t^{(z)} \quad (22c)$$

where a , b and ε are suitable constants and $\eta_t^{(x)}$, $\eta_t^{(y)}$, $\eta_t^{(z)}$ are independent, delta-correlated Gaussian variables with zero mean and unitary variance. In this model the dynamics of y_t and z_t is influenced by x_t , which feels in turn the effect of y_t because of the feedback term εy_t in the r.h.s. of Eq. (22a). A sketch of the interaction scheme is shown in the inset (a) of Fig. 1.

The main plot in Fig. 1 shows the time dependence of the response function between y_t and z_t . As it is clear from the structure of the dynamics, after one time step there is no causal influence (an external perturbation of y_t does not reflect on z_{t+1}). At subsequent times the dynamics of z_t is altered by the perturbation, and the value of the response function crucially depends on the feedback parameter ε , as expected. Due to the linearity of the model, Eq. (13) can be simplified into [3]:

$$R_t = C_t C_0^{-1} \quad (23)$$

where C_t represents the correlation matrix at time t , i.e. $C_t^{ij} = \langle x_i(t) x_j(0) \rangle$ (with $x_1 = x, x_2 = y, x_3 = z$), and C_0^{-1} is the inverse of C_0 . The linearity of Eqs. (22) implies that P_{st} is a multi-variate Gaussian and this immediately leads to Eq. (23). Exploiting this version of the generalized FDR, as shown in Fig. 1, one can estimate $R_{zy}(t)$ from a

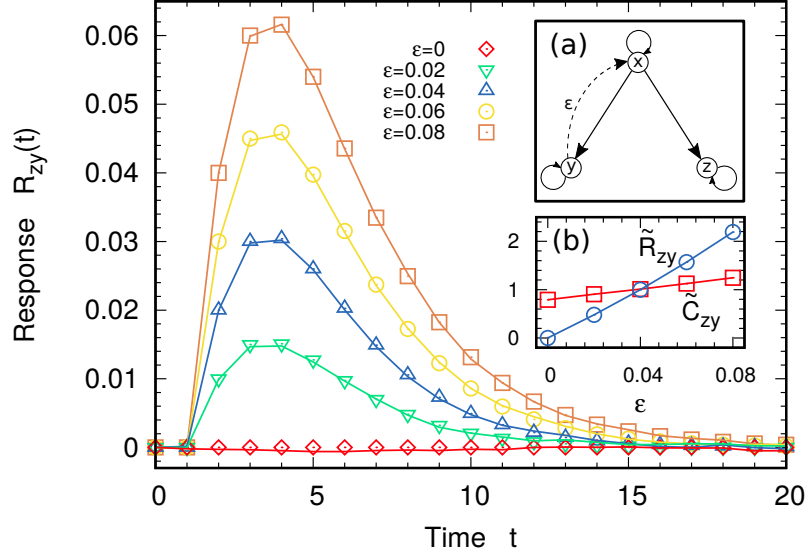


Fig. 1 Relation between causation and response. Main plot: response matrix element $R_{zy}(t)$ of model (22), as a function of time, for several values of the feedback parameter ϵ ; numerical simulations in which the system is actually perturbed (points) are compared to the predictions of the generalized FDR (13) (lines). Inset (a): scheme of the interactions occurring in model (22). Inset (b): correlations (red squares) and responses (blue circles) integrated over time, as functions of ϵ ; both quantities are rescaled with their values at $\epsilon = 0.04$ for graphical convenience. Parameters: $a = 0.5$, $b = 1$. Perturbation for the computation of response: $\delta y_0 = 0.01$. $M = 10^6$ trajectories have been considered for the averages.

suitable combination of correlation functions: the agreement with the actual responses, computed from numerical simulations, is excellent.

It is worth noticing that the mere knowledge of $C(t)$ is not at all informative about the causal links among the elements of the system. For the considered model this fact can be qualitatively appreciated by looking at inset (b) of Fig. 1, where we compare the behavior of $\tilde{R}_{zy} = \int_0^\infty R_{zy}(t) dt$ and $\tilde{C}_{zy} = \int_0^\infty C_{zy}(t) dt$ as functions of ϵ : while the former quantity, in the considered $\epsilon \ll 1$ regime, is almost proportional to ϵ , the latter does not crucially depend on the feedback parameter and it is different from zero also for $\epsilon = 0$. This difference is clearly due, in the considered example, to the common dependence of y_t and z_t on the variable x_t , inducing a “spurious” correlation between the two (meaning that such a correlation does not unveil any causal link between the two processes).

Using the generalized FDR is not the only way to get some insight into the causal structure of a physical system without perturbing its dynamics. A widely employed method is due to Granger [46] and relies on the computation of the forecasting uncertainty for a given variable of a system, using linear regression models; if it is possible to improve the prediction’s precision by including in the model a second, different variable of the system, one may assume a cause-effect relation between the two. A different approach (which has been shown to be equivalent to Granger’s method in the case of linear dynamics [42, 47]) is based on the analysis of information transfer between the variables, a process quantified by the so-called *transfer entropy* and by other related observables [48, 49, 50, 51]. Despite the useful information provided by these approaches, response functions appear to be more accurate in characterizing causal relations, at least from a physical point of view; indeed they quantify the (average) consequence of an actual intervention on the system, at variance with Granger’s method and transfer entropy analysis, which face the problem from the point of view of predictability and uncertainty [52, 53, 45, 54]. In this respect, generalized FDRs as Eq. (13) are, to the best of our knowledge, the only way to deduce the causal structure of a system, in a proper physical sense, by only observing its spontaneous evolution.

3.2 Spin and disordered systems

Here we focus on some applications of the FDR in the contexts of spin models and disordered systems. As already underlined, the main aim of an FDR is to give a tool to calculate a response without applying the perturbation. The direct calculation of a linear response function, for instance in numerical simulations (but the same can be true for experiments), is a very time-demanding task: indeed, the signal fluctuations generally increase when the applied field is small, a condition required for the linear regime to hold. Therefore, the application of FDRs in numerical computations is an effective shortcut to get information on the response function from the measure of the correlations in the unperturbed state. This shortcut has been frequently used to develop field-free algorithms in the context of spin systems [55, 56, 57, 40, 58], and glasses [59] or active matter [60]. Let us note that, at variance with previous attempts, specifically designed for a numerical implementations [56, 57, 59], the FDR reported in Eq. (19) involves the quantity B defined in (20), which is an observable quantity because only depends on the state of the system at a given time and therefore can be in principle measured in real experiments.

3.2.1 Non-linear FDRs

The FDRs in the form (19) can be also derived at nonlinear orders in the perturbation, involving multi-point correlation functions. Non-linear response functions play a central role in the context of glassy systems [61, 62, 63, 64], where usually two-point correlators remain always short-ranged due to the presence of disorder. In particular, in a spinglass the linear susceptibility does not diverge at the critical temperature, whereas non-linear susceptibilities show a divergence when the low temperature phase is approached, signaling a growing amorphous order in the system. Therefore, the relation between nonlinear responses and multi-point correlation functions can be an important tool in the context, as initially proposed in [65]. A general derivation of nonlinear FDRs valid for arbitrary order was presented in [66, 41]. We report here the form of the second-order response for spin variables perturbed by two fields \mathcal{F}_1 and \mathcal{F}_2 at sites j_1 and j_2 at times t_1 and t_2 [41]

$$\begin{aligned} R_{O\mathcal{F}}^{(2)}(t, t_1, t_2) &\equiv \frac{\delta\langle O(t) \rangle_{\mathcal{F}}}{\delta\mathcal{F}_1(t_1)\delta\mathcal{F}_2(t_2)} \Big|_{h=0} \\ &= \frac{1}{4T^2} \left\{ \frac{\partial}{\partial t_1} \frac{\partial}{\partial t_2} \langle O(t) \sigma_{j_1}(t_1) \sigma_{j_2}(t_2) \rangle - \frac{\partial}{\partial t_1} \langle O(t) \sigma_{j_1}(t_1) B_{j_2}(t_2) \rangle \right. \\ &\quad \left. - \frac{\partial}{\partial t_2} \langle O(t) B_{j_1}(t_1) \sigma_{j_2}(t_2) \rangle + \langle O(t) B_{j_1}(t_1) B_{j_2}(t_2) \rangle \right\}. \end{aligned} \quad (24)$$

Let us note that at equilibrium, exploiting the property (21), Eq. (24) simplifies to

$$R_{O\mathcal{F}}^{(2)}(t, t_1, t_2) = \frac{1}{2T^2} \left\{ \frac{\partial}{\partial t_1} \frac{\partial}{\partial t_2} \langle O(t) \sigma_{j_1}(t_1) \sigma_{j_2}(t_2) \rangle - \frac{\partial}{\partial t_2} \langle O(t) B_{j_1}(t_1) \sigma_{j_2}(t_2) \rangle \right\}, \quad (25)$$

with $t > t_1 > t_2$. Therefore, the presence of the model-dependent quantity B is not canceled, making the higher order FDRs somehow less general than the linear one. As suggested in [67] and [68] this observation can provide information on the dynamical rules governing the system from the study of the equilibrium nonlinear responses.

Other interesting applications of nonlinear FDRs are related to the study of the thermal response of the system (namely, a perturbation applied to the noise intensity) as discussed in [69], or in the wide field of nonlinear optics and quantum spectroscopy [70, 71].

3.2.2 Effective temperature

One of the main theoretical applications of the FDRs is the possibility to introduce an effective temperature, from the ratio between response and correlation. Review articles on this interesting subjects are [72, 27, 12, 73, 74]. Here we illustrate such a concept for a spin system, where the linear susceptibility, using the FDR (19), can be written as

$$\chi(t, t_w) \equiv \int_{t_w}^t ds R_{\sigma\mathcal{F}}(t, s) = \frac{\beta}{2} \int_{t_w}^t ds \left[\frac{\partial}{\partial s} C(t, s) - \langle \sigma_i(t) B_i(s) \rangle \right], \quad (26)$$

where $C(t, s) = \langle \sigma_i(t) \sigma_i(s) \rangle$ and t_w is a reference waiting time. Observing that the quantity

$$\psi(t, t_w) = \int_{t_w}^t ds \frac{\partial}{\partial s} C(t, s) = 1 - C(t, t_w), \quad (27)$$

for fixed t_w , is a monotonously increasing function of time, one can reparametrize t in terms of ψ and write $\chi(\psi, t_w)$.

In equilibrium, there is no dependence on the waiting time t_w and one obtains a linear parametric representation

$$\chi(\psi) = \beta\psi, \quad (28)$$

yielding

$$\beta = \frac{d\chi(\psi)}{d\psi}. \quad (29)$$

Out of equilibrium, a nonlinear dependence can arise and an effective temperature can be introduced generalizing Eq. (29)

$$\beta_{eff}(\psi, t_w) = \frac{\partial \chi(\psi, t_w)}{\partial \psi}, \quad (30)$$

with $\beta_{eff} = 1/T_{eff}$. Then one can define a Fluctuation-Dissipation ratio with respect to the temperature T of the dynamics (after the quench)

$$X(\psi, t_w) = \frac{T}{T_{eff}(\psi, t_w)}. \quad (31)$$

which represents a measure of the deviation from equilibrium. In the limit of large waiting time, the functional dependence of X on the correlation function can show different behaviors, shedding light on the relevance of different characteristic time-scales in the system. A detailed discussion of this quantity in the context of aging and glassy systems can be found in [55]. More recent applications of the FDR to equilibrium and non-equilibrium properties of spin glasses have been reported in [75].

The concept of effective temperature has been also applied to systems in the stationary state, such as driven granular media or active particles (see for instance [76, 77]). In this case, the problem is to understand the meaning and the role played by the effective temperature. In some situations, usually when the system is gently driven and the entropy production flux is small, the relevant features of the system behavior can be successfully interpreted in terms of this parameter, leading to an equilibrium-like description. In other cases, the effective temperature can represent an evocative or appealing concept, but does not significantly help in the understanding of the underlying physical mechanisms, see next Section.

3.3 Granular materials

Granular materials appear in our everyday life and in several industrial applications, posing deep questions to statistical physics and technology [78, 79, 80, 81]. A granular medium is an ensemble of macroscopic “grains”, which interact (among each other and with the surroundings) through non-conservative forces. Several orders of magnitude separate the average energy of internal thermal fluctuations at room temperature - $k_B T \sim 5 \cdot 10^{-21} J$ - and the macroscopic energy of a grain (e.g. that related to the position and motion of center of mass): for instance $mgr \sim 10^{-5} J$ for a steel sphere with $r = 2mm$, g being the gravity acceleration. Granular media can display “phase” behaviors: when diluted and under strong shaking a granular “gas” is realised, but when allowed volume and/or the intensity of shaking are reduced, the granular system behaves as a dense “liquid” or a slowly deforming “solid” [82]. The slow-dense phase, close to the so-called *jamming* transition, is difficult to be analysed: we refer the reader to different theoretical approaches [83, 84, 85, 86, 87, 88, 89, 90, 91, 92]. We briefly summarise the more clear situation established for granular gases and liquids.

A granular gas is realized when the packing fraction is small, typically of the order of 1% or less, such that one can assume instantaneous inelastic binary collisions with restitution coefficient $\alpha \leq 1$ (the value 1 is for elastic collisions). In experiments, usually done under gravity, it is necessary to shake the container with accelerations much larger than gravity in order to keep the packing fraction small everywhere [93, 94, 80, 81]. The three main categories of gas regimes are: 1) cooling granular gases, non-steady states which are initially prepared as at equilibrium, and leaving the total energy dissipate under repeated inelastic collisions [95, 96, 97]; 2) boundary driven gases, where at least one wall injects energy into the gas (e.g. vibration in experiments, thermostats in theory), reaching a non-homogeneous steady state [98, 99, 100]; 3) bulk driven granular gases, where each particle is in repeated contact with some source of energy, for instance bouncing above a vibrating rough plate [101, 102, 103, 104, 105], reaching a homogeneous steady state.

In granular gases it is customary to define a kinetic “granular temperature” [106, 107, 108, 109]

$$k_B T_g = \frac{m \langle |\mathbf{v}|^2 \rangle}{d}, \quad (32)$$

with \mathbf{v} the velocity of each particle, d the dimensionality of space and k_B is usually replaced with 1. Such a temperature is not expected to have a wide thermodynamic meaning, and also in statistical mechanics it has not a role equivalent to that played for molecular gases, for instance deviations from a Maxwellian are inevitable in the presence of inelastic collisions, a kurtosis excess (or second Sonine coefficient) is observed - larger or smaller - in many regimes [97, 110]. In all gas and liquid regimes, moreover, there is no equipartition of energy among different degrees of freedom (e.g. in a mixture or under non-isotropic external forces), unless they have identical properties [111, 112, 113, 114, 115, 116, 117, 118].

Linear response relations have been frequently studied for granular gases and liquids, particularly in steady states [119, 120, 121, 122, 123, 124, 125, 126, 127, 39], while a few studies also considered cooling regimes [128, 120, 125]. In dilute homogeneously driven granular gases, the equilibrium FDR is empirically observed, provided that the canonical temperature is replaced with the tracer granular temperature T_0 which - in general - can be different from T_g [119, 121, 122, 126, 127]. For instance, a granular tracer under the action of a weak perturbing force in a dilute driven granular system satisfies the dynamical Einstein relation, Eq. (4) with $T = T_0$. Such a result is surprising as, on the basis of the FDR discussed above, Eq. (13) and of the non-Gaussian distribution of velocities, one would expect a correction to it. Nevertheless, in many different dilute cases, such corrections are not observed or - in certain solvable models - can even be proven to vanish [127]. A possible explanation to such a general result comes through the *molecular chaos* which is likely to be valid in dilute cases and which implies that a particle 1 meets particle 2 only once: any collision rule, if restricted to a single particle (that is, disregarding the fate of particle 2) is equivalent to an *elastic* collision with effective masses [12]. For a massive intruder (mass much larger than the other particles), the validity of the Einstein relation is recovered in the context of the derivation of an effective Langevin equation model [129]

The liquid (non dilute) case is perhaps more interesting. The first experiment focusing on a Brownian-like description of a large intruder in a granular liquid is discussed in Ref. [130]. Most recent studies, both theoretical [124, 126, 127, 131, 132] and experimental [39], have shown that when the granular is a liquid and not a gas, deviations from the equilibrium Fluctuation-Dissipation relation are observed. In granular liquids, as a matter of fact, granular temperature is much less useful than in gases, and cannot be replaced by some other temperature for the purpose of an effective description.

An interesting example, in theory and in experiments is provided, again, by a massive intruder $M \gg m$ [131, 132]. For the purpose of describing, in numerical simulations, the autocorrelation of the velocity V of the tracer and its linear response, the following model provides a fair description for packing fractions smaller than 40%:

$$M \dot{V}(t) = -\Gamma[V(t) - U(t)] + \sqrt{2\Gamma T_{tr}} \mathcal{E}_V(t) \quad (33a)$$

$$M' \dot{U}(t) = -\Gamma' U(t) - \Gamma V(t) + \sqrt{2\Gamma' T_b} \mathcal{E}_U(t), \quad (33b)$$

where $U(t)$ is an auxiliary variable representing the memory effect due to the average velocity field of the particles surrounding the tracer, Γ and T_{tr} are the effective drag coefficient and tracer temperature (both can be derived by kinetic theory in the dilute limit), Γ' and M' are parameters to be determined, for instance from the measured autocorrelation function, and T_b is the value of T_g in the elastic limit (for instance the external bath temperature [102]). Equations (33) can be mapped into a generalised Langevin equation, Eq. (11), with exponential

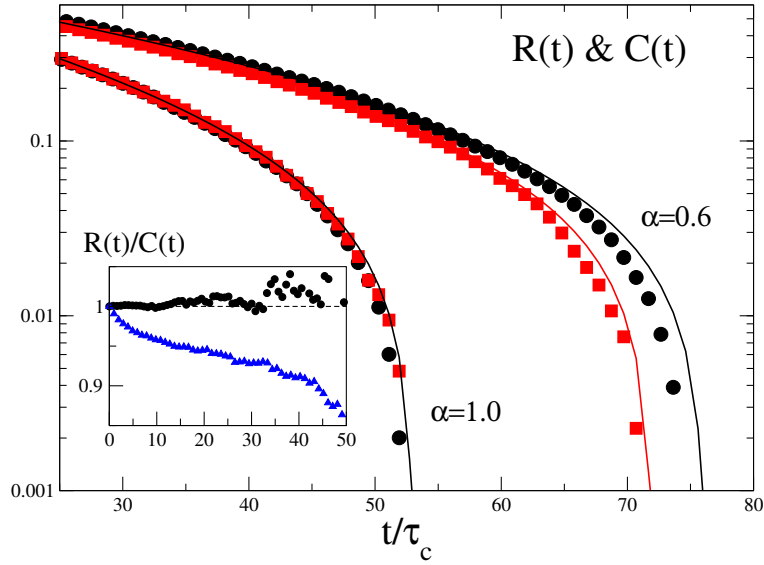


Fig. 2 Response function of the tracer’s velocity V under a perturbing force F , $R_{VF}(t)$ and auto-correlation function $C(t) = \langle V(t)V(0) \rangle / \langle V(0)V(0) \rangle$ as a function of time, measured in molecular dynamics simulations of a system composed of a massive intruder interacting with a driven granular fluid [131]. In the main plot an elastic case with restitution coefficient $\alpha = 1$ (where the two functions superimpose as in equilibrium FDR) and an inelastic case $\alpha < 1$ (where equilibrium FDR is violated) are shown. In the inset the ratio between the two curves is shown for the two cases (black is elastic, blue is inelastic).

memory kernel. In the dilute limit (parameters such that U is negligible) the massive tracer evolves according to a simple Langevin equation. In the elastic limit ($T_{tr} = T_b = T_g$), on the other side, the coupling with U is still important, but the equilibrium Fluctuation-Dissipation relation is recovered. The numerical simulations have shown that the auxiliary field $U(t)$ is a local average of the velocities of the particles surrounding the intruder. When the density increases numerical simulations suggest $T_{tr} \rightarrow T_g$, likely due to a reduction of effective inelasticity in recolliding particles. The appearance of T_b is also interesting: the “temperature” associated to the local velocity field U is equal to the bath temperature and this seems a consequence of the conservation of momentum in collisions, implying that the average velocity of a group of particles is not changed by collisions among themselves and is only affected by the external bath and a (small) number of collisions with outside particles. Summarizing, model (33) suggests that in a granular liquid - at some level of approximation - *two* temperatures are relevant, one related to the single particle scale and another one related to a many-particle, or collective, scale. Such a conclusion is consistent with a series of recent results about spatial velocity correlations, typically measured as structure factors of the velocity field [133, 134, 135, 136, 137, 101, 104, 138, 105, 139, 140].

3.4 Application to biological systems and active particles

The results of the FDR have been also applied to several biological systems, for instance in an evolution experiment in bacteria [141] or in the prediction of heart rate response [142]. Another recent application has been proposed in the context of brain activity. Indeed, one can wonder whether, at some scale, the evoked activity in the brain to an external stimulus can be somehow predicted from the observation of the spontaneous, rest activity. In order to quantitatively address this issue, one needs an effective model to describe the brain dynamics at the considered scale. In the work [143], the authors considered the stochastic version of the Wilson-Cowan model [144], describing at a coarse-grained level the dynamics of populations of excitatory and inhibitory neurons. In the linearized version, this model consists in two coupled linear Langevin equations for the two populations. The prediction of the FDR for this model was compared to experimental Magnetoencephalography (MEG) data for rest and evoked activity in healthy subjects. Whereas the behavior of the temporal autocorrelation function of the total rest activity (excitatory plus inhibitory neurons) showed a double exponential decay characterized by two typical times, the decay of the

response function was described by a single exponential decay, in qualitative agreement with the prediction of the FDR. These results suggest that some information of the brain response to external stimuli can be obtained from the observation of its spontaneous activity.

A different field which is in large part contained in biology and biophysics, is that of self-propelled particles, where non-equilibrium stochastic dynamics has been employed as a main modelling tool [145, 146]. These systems, known as “active”, are usually out of equilibrium and store energy from the environment, for instance taking advantage of chemical reactions or mechanical agents (such as bacterial cilia and flagella), to produce directed motion [147]. The intrinsic non-equilibrium nature of the class of models proposed to describe active systems makes them the ideal platforms to test any version of the generalized FDR [148, 149]. Since their steady-state properties are quite rich, involving unexpected spatial correlations in density, velocity and polarization fields, the use of Eq. (13) can be challenging. For this reason, this method has been applied only in the limit of small activity [150] when the steady probability distribution is known perturbatively or using effective equilibrium-like approaches. This allows one to derive a near-equilibrium expression for the susceptibility [151] and approximated predictions for the transport coefficients of active particles, such as their mobility [152]. In addition, the Malliavin weight sampling has been recently generalized to the more common models used to describe the active particle dynamics [60]. This technique was particularly useful to explore numerically far from equilibrium regimes, calculating i) the mobility of an interacting active system at low density [152] ii) the response function due to a shear flow [153] and, finally, iii) the active effective temperature [154, 155, 156, 157].

In this section, going beyond the approximated approaches explained so far, we apply the technique reported in Sec. 2.2 to obtain exact expressions for the generalized FDR valid in active matter systems [158, 38]. Specifically, we focus on particle systems in the framework of dry active matter without momentum conservation. In this context the evolution of an active particle of mass m is described by a set of stochastic equations for its position, \mathbf{x} , and its velocity, \mathbf{v} , given by [159, 160]:

$$\dot{\mathbf{x}} = \mathbf{v} \quad (34a)$$

$$m\dot{\mathbf{v}} = -\gamma\mathbf{v} - \nabla U + \mathbf{f}^a + \sqrt{2T\gamma}\boldsymbol{\eta}, \quad (34b)$$

while, in the more common overdamped version, such that $m/\gamma \ll 1$, reads:

$$\gamma\dot{\mathbf{x}} = \mathbf{F} + \mathbf{f}^a + \sqrt{2T\gamma}\boldsymbol{\eta}. \quad (35)$$

In both the dynamics, \mathbf{f}^a is a non-gradient force, called “active force” for simplicity, that models at a coarse-grained level the system-dependent mechanism responsible for the active dynamics so that its complex physical or biological origin is not explicitly considered. This term is chosen as a time-dependent force that provides a certain degree of persistence to the particle trajectory in agreement with the experimental observations of active colloids, bacteria, and other biological microswimmers. The most popular models to account for this persistence in the framework of continuous stochastic processes are the Active Brownian Particles (ABP) [161, 162, 163, 164, 165, 166, 167] and the Active Ornstein-Uhlenbeck particles (AOUP) [168, 169, 170, 171, 172, 173]. In both cases, the active force is expressed as:

$$\mathbf{f}^a = \gamma v_0 \mathbf{n}, \quad (36)$$

where v_0 is the swim velocity induced by the active force and \mathbf{n} is a vector representing the particle orientation that evolves stochastically. In the ABP model, \mathbf{n} is a unit vector that evolves as

$$\dot{\mathbf{n}} = \sqrt{2D_r}\mathbf{n} \times \boldsymbol{\xi}, \quad (37)$$

while in the AOUP model, \mathbf{n} follows an Ornstein-Uhlenbeck process with unitary variance:

$$\tau\dot{\mathbf{n}} = -\mathbf{n} + \sqrt{2\tau}\boldsymbol{\xi}. \quad (38)$$

In both equations, $\boldsymbol{\xi}$ is a vector of δ -correlated white noises with zero average. The coefficient D_r is the rotational diffusion coefficient while τ is simply named persistence time since it coincides with the autocorrelation time of the active force. The models reproduce consistent results by choosing $(d-1)D_r = 1/\tau$ where $d > 1$ is the dimension of the system [164].

In general, the active force pushes the system out of equilibrium, producing entropy with a rate that grows with τ [174, 175, 176, 177, 178]. Applying Eq. (17) to the dynamics (34), the elements of the response matrix after perturbing the x component of the velocity, read [38]:

$$\mathcal{R}_{v,v}(t) = \frac{m}{T} \langle v(t)v(0) \rangle + \frac{m}{2T\gamma} (\langle v(t)\nabla_x U(0) \rangle + \langle \nabla_x U(t)v(0) \rangle - \langle v(t)f^a(0) \rangle - \langle f^a(t)v(0) \rangle) \quad (39a)$$

$$\mathcal{R}_{x,v}(t) = \frac{m}{2T} \langle x(t)v(0) \rangle + \frac{m}{2T\gamma} \langle x(t)\nabla_x U(0) \rangle - \frac{m}{2T\gamma} \langle x(t)f^a(0) \rangle - \frac{m^2}{2T\gamma} \langle v(t)v(0) \rangle, \quad (39b)$$

where we have suppressed the spatial indices for simplicity. Equation (39a) is determined by the generalized retarded kinetic energy and the time-symmetric retarded power injected by the gradient force and the active force. In Eq. (39b), we can identify the retarded mechanical pressure (second term), the so-called retarded swim/active pressure (third term) and, finally, the retarded/anticipated kinetic energy (fourth term). Applying Eq. (17) to the dynamics (35), the response after perturbing the coordinate x of the particle position reads [38]:

$$\mathcal{R}_{x,x}(t) = \frac{1}{2T} (\langle x(t)\nabla_x U(0) \rangle + \langle \nabla_x U(t)x(0) \rangle) - \frac{1}{2T} (\langle x(t)f^a(0) \rangle + \langle f^a(t)x(0) \rangle). \quad (40)$$

In the overdamped case, the response is determined by the sum of the time-symmetric part of the retarded/anticipated mechanical and swim pressures. In overdamped systems with $T = 0$, the above formulation of the FDR cannot be directly applied, because the dynamics is not of the Langevin form. In this athermal case, another version of the generalized FDR can be derived using a modified path-integral method developed in [158] in the case of AOUP (FDR for athermal ABP are still unknown), obtaining:

$$D_a \gamma \mathcal{R}_{x,x}(t) = \frac{1}{2} [\langle x(t)\nabla_x U(0) \rangle + \langle \nabla_x U(t)x(0) \rangle] + \frac{\tau^2}{2} \sum_{\alpha} [\langle v_{\alpha}(t)\nabla_{\alpha}\nabla_x U(t)v_x(0) \rangle + \langle v_x(t)\nabla_x\nabla_{\alpha} U(0)v_{\alpha}(0) \rangle], \quad (41)$$

where we have introduced the particle velocity $v_{\alpha} = \dot{x}$, with $\alpha = x, y$. According to our notation, repeated indices are summed, $U(s) = U(\mathbf{x}(s))$. The first line of Eq. (41) coincides with the equilibrium FDR holding for passive particles where the detailed balance holds. The second line contains two additional terms, involving the particle velocity and the second derivative of the potential, that disappears in the equilibrium limit $\tau \rightarrow 0$. At variance with the equilibrium scenario, in athermal active systems, the generalized FDR is not only determined by a time correlation involving the position but is affected by the correlations between the other variables, such as the velocity.

To validate the generalized FDR in the case of active particles, we consider both AOUP and ABP dynamics confining the particle through a non-linear force due to an external potential. To go beyond the harmonic case that can be solved analytically [158], we chose a quartic potential, $U(\mathbf{x}) = k|\mathbf{x}|^4/4$, where the constant k determines the strength of U . In Fig. 3, we show the diagonal elements of the response matrix numerically obtained by their definitions (i.e. perturbing the dynamics) and the FDR numerically calculated from the unperturbed system. In particular, in panel (a), we show the results in the underdamped case, reporting the profile of $R_{v,v}(t)$ and the FDR calculated from Eq. (39a), while, in panel (b), the analogue study is reported for the overdamped dynamics, comparing $R_{x,x}(t)$ and the FDR, Eq. (40). In both cases, the FDRs exactly match with the direct study of the response confirming the exactness of our theoretical results. Finally, in the inset of panel (b), we compare Eq. (40) in the limit of small temperature, T , and the athermal relation, Eq. (41). We reveal that the former converges onto the latter for $T \rightarrow 0$.

4 Conclusions

We have reviewed two significant approaches to the problem of linear response in general systems, when the constraint of thermodynamic equilibrium for the unperturbed state is removed. We have also sketched some of the interesting recent applications of such approaches. We cannot avoid to stress, again, the evident fact that - given the system, the observable of interest and the applied perturbation - the linear response function is unique and

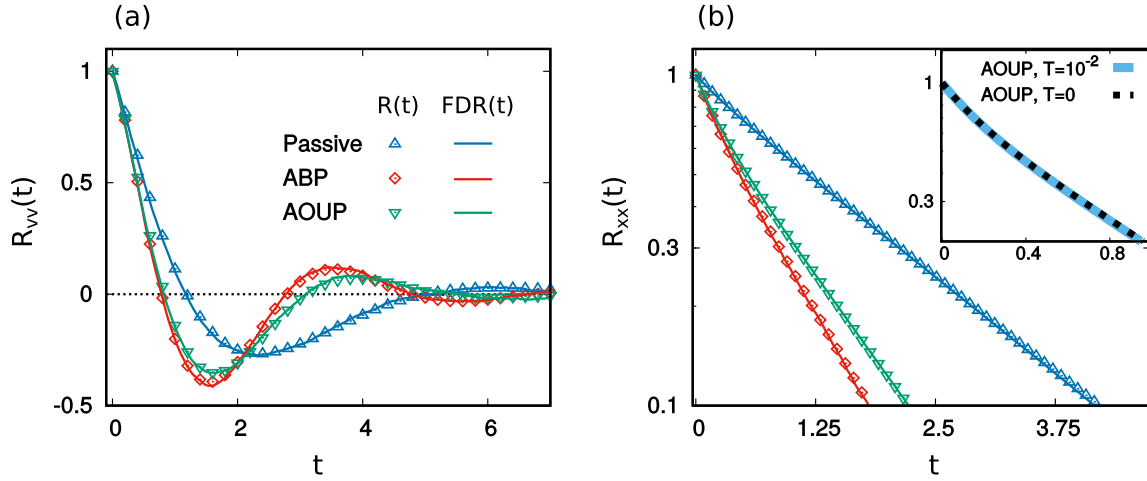


Fig. 3 Comparison between response and FDR for a two-dimensional particle confined in a quartic potential, $U(\mathbf{x}) = k|\mathbf{x}|^4$. Panel (a): $R_{vv}(t)$ (colored points) calculated perturbing the velocity of the underdamped dynamics, Eq. (34). Panel (b): $R_{xx}(t)$ (colored points) calculated perturbing the position of the overdamped dynamics, Eq. (35). The responses are shown for passive, ABP and AOUP as explained in the legend which is shared by both panels. Solid color lines plot the FDR, obtained using Eq. (39a) and (40), for panels (a) and (b), respectively. The inset of panel (b) shows a comparison between Eq. (40) (calculated at $T = 10^{-2}$) and Eq. (41) (holding for $T = 0$). The other parameters of the simulations are $k = 3$, $\gamma = 1$, $T = 10^{-1}$, $v_0 = 1$, and $\tau = 1$.

therefore the two approaches lead to the same result, and in fact an analytical connection can be demonstrated [179]. The difference between the two schemes relies on the required information: in one case, formula (13), one needs some knowledge about the probability distribution at initial time (e.g. the steady-state one) for the relevant degrees of freedom; in the other case, formulas (14), (17) and (19), one needs knowledge about the system's dynamical model (e.g. noise distributions, forces involved, transition rates, etc.). It is not always evident when one approach is more useful than the other. In lucky cases, where both the dynamical model and its probability distribution are known, the two formulas can express different information and one can be more useful than the other (for instance correlations with state variables can be more transparent than correlations with noises or time-derivative of state variables).

In experimental situations, where the underlying model is not known, an empirical approach to retrieve the main features of the probability distribution of the relevant degrees of freedom can be simpler than retrieving information about forces and noises in the system, suggesting the first approach as the more useful. If a dynamical model is known for the relevant degrees of freedom, while the generated probability distribution is unknown, then the second approach should be more direct. However it is clear that, even when a dynamical model is fully available, the first approach may have some advantage: for instance, in a system with many particles and a massive tracer whose response is investigated, the knowledge of the dynamics of all the particles can be too detailed and result, when inserted in the second approach, in quite a complicate formula, or even not very informative and/or transparent ones; an empirical study of the probability distribution of the relevant degrees of freedom (e.g. those of the tracer and some coarse-grained observable for the surrounding fluid) can provide, sometimes, an approximate but more informative route through the first approach (see for instance the example discussed in Section 3.3).

We also recall that an FDR does not give an explicit prediction for the response, but only an expression of it in terms of unperturbed correlations. Once an FDR is known, the problem of obtaining (empirically or analytically) the required correlations remains. An FDR however can have already a theoretical meaning, even without the explicit knowledge of the time-dependence of the involved unperturbed correlations, i.e. it is already significant to know *which* correlations are involved, as well illustrated by the application described in subsection 3.1 for the problem of causation and also in the closure problem in the Kraichnan's approach to turbulence [1].

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