Fluctuation-dissipation relations for steady-state systems

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Abstract – The fluctuation-dissipation (FD) theorem is a fundamental result for systems near thermodynamic equilibrium. It states that the nonequilibrium relaxation dynamics is related to the spontaneous fluctuation at equilibrium. Recently we have shown that the dynamics of a dissipative system described by stochastic differential equations can be mapped to that of a thermostated Hamiltonian system, with a nonequilibrium steady state of the former corresponding to the equilibrium state of the latter. In present manuscript, the corresponding FD theorem is derived in the way parallel to the procedure for deriving the near equilibrium FD theorem, based on this mapping. The analytical results in the present approach are in good agreement with numerical results. We find some previous results are special cases of the current relations. We also suggest further studies exploiting the analogy between a general dissipative system appearing in other science branches and a Hamiltonian system.

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Introduction. – It is ubiquitous to observe a system at a state invariant with time (with the approximation that the relevant constraining parameters changes much slower than the time scale under interest). It can be a thermodynamic equilibrium state, or more likely a nonequilibrium steady state. Some examples are homeostatic states of living organisms, a stable eco- or financial system. Quite often it is important to know how a system initially subject to a perturbation relaxes to a steady state (including the equilibrium state) after removal of the perturbation. The fluctuation-dissipation (FD) theorem states that the relaxation dynamics for a process close to equilibrium is related to the spontaneous fluctuation at equilibrium. Originally formulated by Nyquist in 1928 [1], and first proved by Callen and Welton in 1951 [2], the FD theorem is related to many important results in statistical physics. Examples are the Einstein-Smoluchowski relation between the diffusion constant and drag coefficient [3,4], Onsager’s regression hypothesis [5,6], and the linear response theory [7]. The FD relation also has practical importance. It allows deducing nonequilibrium dynamics from equilibrium measurements, and justifies the relation between macroscopic dynamics and microscopic level simulations, e.g., calculating the diffusion constant. In recent years, fluctuation theories of nonequilibrium processes, especially for systems far from equilibrium received great attention [8–19].

On studying problems from physics, chemistry, cellular biology, ecology, engineering, finance, and many other fields, the following form of Langevin equations is widely used [20–22]:

\[ dx_i/dt = G_i(x) + \sum_{j=1}^{m} g_{ij}(x) \zeta_j(t), \quad i = 1, \ldots, n. \quad (1) \]

In general, \( m \) and \( n \), the number of row and column of matrix \( g \) may be different, \( \zeta_i(t) \) are temporally uncorrelated, statistically independent Gaussian white noise with the correlation satisfying \( \langle \zeta_j(t) \zeta_j'(t') \rangle = \delta_{j,j'} \delta(t-t') \). The stochastic term in eq. (1) can reflect both additive noise and multiplicative noise of the system. The \( g(x) \) is related to the \( n \times n \) diffusion matrix \( D \) by \( gg^T = 2D/\beta \), where

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the “T” refers to the transpose of a matrix. For a physical system \( \beta = 1/k_B T \). For a non-physical system, one can define an effective temperature relating to \( \beta \). Recently we have proven that there exists a mapping between a stochastic dissipative system described by eq. (1) and a thermostated Hamiltonian system [23]. The mapping allows many results from equilibrium statistical physics directly applicable to nonequilibrium processes. Specifically in this work, we will derive the FD relation applicable to processes far from equilibrium. An FD relation, if exists, would allow predicting the relaxation dynamics to a steady state through measurements of steady-state fluctuations. The latter are in general easier to measure.

**Theory.** – In ref. [23], we showed how to map the dynamic system described by eq. (1) to a Hamiltonian system in the zero-mass limit,

\[
H = \left( \frac{p - A(q)}{2m} + \phi(q) + H_b(q,p,Y) \right). 
\]

with

\[
H_b = \sum_{\alpha} \sum_j \left[ \frac{1}{2} \omega_{\alpha j}^2 (q_{\alpha j} - a_{\alpha}(q))/(\sqrt{N} \omega_{\alpha j}^2) \right] ,
\]

provided that the system possesses a stationary distribution. The terms \( \phi(q) \) and \( A(q) \) are scalar and vector potentials, respectively. The term \( H_b \) is a type of bath Hamiltonian discussed by Zwanzig [24]. The Hamiltonian mathematically describes a particle, coupled to a set of harmonic oscillators, moving in a hypothetical dimensional conservative scalar potential and magnetic field (described by the vector potential).

Here we briefly summarize the mapping work. For a stochastic system described by eq. (1), Ao et al. [14,15] developed a \( S + T \) transformation technique,

\[
(S + T) \cdot \frac{dq}{dt} = (S + T) \cdot (G(q) + g(q) \cdot \zeta(t)) = -\nabla_q \phi(q) + g'(q) \cdot \zeta(t),
\]

where \( \phi(q) \) is a scalar function corresponding to the potential function in the Hamiltonian system.

At the zero-mass limit, the equations of motion (EOMs) of the Hamiltonian system shown in eq. (2), are exactly eq. (3). In eq. (3), the terms \( \nabla_q \phi(q) \) and \( Td\zeta dt \) come from the EOM of Hamiltonian \( (p - A(q))/2m + \phi(q) \), (with \( T_{ij} = \partial A_{ij} / \partial \eta_{ij} - \partial A_{ij} / \partial \eta_{ij} \)), while the terms \( Sdq/dt \) and \( g'(q) \zeta(t) \) are derived from the EOMs of both bath Hamiltonian \( H_b \). This is the key idea of our mapping approach from a stochastic dissipative system to a thermostat Hamiltonian system, which allows many useful results for equilibrium statistic physics directly applicable to nonequilibrium system.

With the mapping, the steady-state distribution of the stochastic system is thus given by the Boltzmann distribution of the corresponding Hamiltonian system,

\[
\rho_{ss}(q) = \frac{\int dp dY \exp(-\beta H(q,p,Y))}{\int dq dp dY \exp(-\beta H(q,p,Y))} = \frac{\exp(-\beta \phi)}{\int dq \exp(-\beta \phi)},
\]

where \( Y \) represents all the bath variables. Equation (4) is also conjectured by Ao [25], and a general proof is given in ref. [26]. It can also be derived from the Fokker-Planck equation constructed from a set of Langevin equations [27].

The steady-state ensemble average of a generic dynamic quantity \( O \) can be described as

\[
\langle O \rangle = \int dq O \rho_{ss}(q).
\]

Consider a system initially at a steady state defined by eq. (1) with an extra infinitesimal perturbation \( \delta G(\lambda(t)) \), where \( \lambda(t) \) refers to the perturbation parameters. At \( t = 0 \), \( \delta G \) is removed, thus the system relaxes to the steady state of \( G \). For the corresponding mapped system, the corresponding Hamiltonian changes from \( H' = H + \delta H = H + (\partial H_{ij} / \partial \lambda_j) \cdot \delta \lambda_i \). Then the nonequilibrium relaxation dynamics of \( O \) follows

\[
\overline{O(t)} - \langle O \rangle \approx \int dq dp \rho(q,p) \exp(-\beta H') - \langle O \rangle \approx -\beta \left\langle O(q) \frac{\partial \phi(q)}{\partial \lambda} \right\rangle - \langle O \rangle \left\langle \frac{\partial \phi}{\partial \lambda} \right\rangle \cdot \delta \lambda(0).
\]

In the above derivation, we used the stationary property of equilibrium ensemble average, so \( \langle O(t) \rangle = \langle O(0) \rangle = \langle O \rangle \). Variation of the bath Hamiltonian makes no contribution. This is the generalized FD relation for systems obeying or violating detailed balance, which states that nonequilibrium relaxation dynamics can be predicted from steady-state fluctuations. If one relates the relaxation function to the linear response function,

\[
\overline{O_{ij}(t)} - \langle O_{ij} \rangle \approx \int_0^t dt' \chi_{ij}(t-t') \delta \lambda_j(t')
\]

one obtains the differential form of the FD relations,

\[
\chi_{ij}(t-t') = -\beta \frac{d}{dt} \left[ \frac{\partial O_{ij}(t)}{\partial \lambda_j} \right].
\]

Equations (6) and (8) are the central results of this work. These results are actually mathematically trivial with the replacement \( \beta \phi = -\ln \rho_{ss} \) [12]. The mapping, however, provides a direct connection between \( \rho_{ss} \) and the Langevin equations, and allows a unified treatment for systems obeying or violating detailed balance. One can generalize the results discussed in this work to higher orders of \( \delta G \), following the approach in ref. [15].
One type of perturbation of special interest is a system coordinate coupled to some constant external force linearly, $\delta \mathbf{H} = \mathbf{f} \cdot \mathbf{q}$, which corresponds to $\delta \phi = \mathbf{f} \cdot \mathbf{q}$. Notice that $\delta \mathbf{G}$ is in general a nonlinear function of $\mathbf{q}$. This situation has been previously discussed by Graham, and by Eyink et al. [28,29]. Under this special type of perturbation, all the familiar results obtained on studying relaxations near an equilibrium state follow [30]. One can define a response function $\chi(t, t')$, so $\mathbf{q}(t) - \langle \mathbf{q} \rangle = \int_{-\infty}^{\infty} dt' \chi(t - t') \mathbf{f}(t') + O(\|\mathbf{f}\|^2)$. The function $\chi(t - t')$ is stationary and satisfies the Kramers-Krönig relations. If $\mathbf{f}$ is time varying with a monochromatic frequency, $\mathbf{f} = \text{Re}[\tilde{f}_0 \exp(i\omega t) + \tilde{f}_0^* \exp(-i\omega t)]$, the system absorbs “energy”, with the absorption spectrum $\text{abs}(\omega) \propto \omega^2 \int_0^\infty dt \mathbf{f}_w^T (\langle \mathbf{q}_t \rangle - \langle \mathbf{q} \rangle) \langle \mathbf{q}_t - \langle \mathbf{q} \rangle \rangle^T \mathbf{f}_w \cos(\omega t)$ [30].

**Examples.** – Obviously if one takes $\mathbf{O}_i = \partial \phi / \partial \lambda_i$, eq. (8) gives the relation derived by Prost et al. from the Hatano-Sasa equality recently [31].

For a simple example, we consider a particle moving along a one-dimensional periodic potential $V(x + L) = V(x)$ and under a constant force $F$. The corresponding Langevin equation is

$$\eta dx/dt = \partial_x V_{eff} + \sqrt{2m/3\zeta(t)}$$

with $V_{eff}(x) = V(x) + F \cdot x$. The “steady-state” distribution (projected to and normalized within a range of $L$) is [32]

$$\rho_{ss}(x) = \mathcal{N} \int_0^L \text{d}x [V_{eff}(x+y) - V_{eff}(x)]/k_bT,$$

where $\mathcal{N}$ is the normalization factor. Compare with the standard form of mapping, we find the corresponding Hamiltonian system can be described by

$$H = \frac{p^2}{2m} + \phi(x) + H_b(q_j, p_j),$$

with $\phi(x) = -\ln \rho_{ss}(x)$, and

$$H_b = \sum_{j=1}^N \left[ \frac{1}{2} \dot{q}_j^2 + \frac{1}{2} \omega_d^2 \left( q_j - \frac{\eta}{N\gamma_{\omega_d} \omega_d} \right)^2 \right],$$

where $\gamma_{\omega_d} \equiv 3\pi/(2\omega_d^2)$, and $\omega_d$ is the cutoff frequency [24]. Then eq. (6) can be rewritten as

$$\mathbf{O}(t) - \langle \mathbf{O} \rangle \approx -\frac{1}{k_bT} \left[ \left( \frac{\partial V_{eff}(x)}{\partial \lambda} \right) - \langle \mathbf{O} \rangle \left( \frac{\partial V_{eff}(x)}{\partial \lambda} \right) \right] \cdot \delta \lambda(0) + \frac{1}{k_bT} \left[ \langle \mathbf{O} \rangle \langle \mathbf{O} \rangle \cdot \delta \lambda(0) \right],$$

where

$$\mathbf{B} = \mathcal{N} \int_0^L \text{d}y \frac{\partial V_{eff}(x + y)}{\partial \lambda} e^{[V_{eff}(x+y) - V_{eff}(x)]/k_bT} \rho_{ss}(x),$$

The second term in the right-hand side of the above equation vanishes when $F = 0$, and so the relation reduces to the FD relation near equilibrium.

Because of the mapping, one can directly apply the standard Kubo linear response formula (see Chapt. 7 of ref. [33]) to systems relaxing to nonequilibrium steady state (NESS),

$$\mathbf{O}_i(t) - \langle \mathbf{O}_i \rangle \approx -\beta \int_0^t \text{d}t' \Phi_{O,i,j}(t') \delta \lambda_j(t' - t),$$

where $\Phi_{O,i,j}(t) = \langle \mathbf{O}_i(t) \partial \phi(x(t))/\partial \lambda_j \langle \mathbf{O}_j \rangle \rangle |_{\tau = 0} = \langle \mathbf{O}_i(t) \partial \phi(x(t))/\partial \lambda_j \rangle |_{\tau = 0}$. Equation (13) is essentially an alternative form of eqs. (7) and (8). For a system under periodic perturbation, within the linear regime, the above equation becomes

$$\Delta \mathbf{O}_i(\omega) = \sigma_{O,i,j}(\omega) \delta \lambda_j(\omega),$$

$$\sigma_{O,i,j}(\omega) = \int_0^\infty \text{d}t \exp(i\omega t) \Phi_{O,i,j}(t)$$

with $\Delta \mathbf{O}_i(\omega) = \int_0^\infty \text{d}t \exp(i\omega t) \mathbf{O}_i(t)$, and $\delta \lambda_j(\omega) = \int_0^\infty \text{d}t \exp(i\omega t) \delta \lambda_j(t)$. Furthermore the Kramers-Kronig relation connects the real and imaginary parts of $\sigma_{O}(\omega)$. A case of special interest is $\mathbf{O}_i(t) = \frac{\partial \phi(x(t))}{\partial \lambda_j}$, One can easily derive a generalization of the Kubo formula of conductivity.

For a special case, $\mathbf{O}(x) = \partial V(x)/\partial \lambda$, and the motion is along a circular track, it remains to be shown whether eq. (13) leads to what derived by Chetrite et al. [34], and experimentally tested by Gomez-Solano et al. [35].

To further test the FD model in nonlinear cases, we considered a model studied by Zhu et al. [36],

$$\frac{d}{dt} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = -\left( \mathbf{S} + \mathbf{T} \right)^{-1} \nabla \phi + \zeta,$$

$$\mathbf{S} = \begin{pmatrix} (q^2 - 1)^2 \\ (q^2 - 1)^2 + 1 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix},$$

$$\mathbf{T} = \begin{pmatrix} (q - 1 + \epsilon)^2 \\ (q^2 - 1)^2 + 1 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

$$\phi = \frac{1}{2} (q - 1)^2,$$

$$\langle \zeta \zeta \rangle = 2D_{ij}/\beta.$$
Simulated
FD
$\Delta x_1(t)$ [R.U.]
0
10
20
30
0
0.5
1
0.5
1
0.4
0.5
0.6
0.9
0.2
0.4
0.6
0.8
1
0.3
0.5
0.7
0.9
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
0.2
0.4
0.6
0.8
1
1
1

Fig. 1: Numerical tests with a model showing limiting cycle dynamics. (a) The normalized relaxation function $\Delta x_1(t) = \frac{x_1(t) - x_1(0)}{(x_1(0) - x_1)}$ from simulation and prediction of the FD relation. $f_1 = f_2 = 0.005$. (b) The "absorption spectrum" calculated from the fluctuation correlation functions with $f_1 = f_2 = 0.005 \cos(\omega t)$. (c) The simulated amplitude of the $x_1$ oscillation driven by an oscillating perturbation used in (b).

Bath Hamiltonian gives

$$H_b = \sum_{\alpha=1}^{N} \sum_{j=1}^{N} \left( \frac{1}{2} \alpha_j^2 + \frac{1}{2} \alpha_j^2 \left( q_{\alpha j} - \frac{\sqrt{D} \alpha_j x_1}{\sqrt{N} \gamma \alpha_j k_B T} \right)^2 \right) \tag{19}$$

Here, $M = S + T$.

In the last expression of eq. (14), the diffusion matrix $D$ is given by the symmetric part of $(S + T)^{-1}$, and we used $\beta = 20$. Compared to what used by Zhu et al., we added an extra term $\epsilon = 0.01$ to avoid singularity at $q = 1$ in the introduced perturbation. $\delta G = (S + T)^{-1} f$, even with elements of the constant vector $f_j \ll 1$. Results in fig. 1(a) show that indeed with this special choice of the perturbation, $\Delta x_1(t) \propto f_1 \langle x_1(t) x_1(0) \rangle + f_2 \langle x_2(t) x_2(0) \rangle$, (noticing $x_1 = 0$), in the linear response regime. This result is striking given that the perturbation $\delta G$ is highly nonlinear. The response function shows damped oscillations. Therefore, one expects van Vleck-Weisskopf-Fröhlich-type resonance absorption [30]. The resonance is confirmed in fig. 1(b). Here we talk about the mapping Hamiltonian. The mapping "energy" is not the same as the physical energy. Nevertheless, one expects that the resonance absorption may manifest itself in the dynamics of $x$ under periodic perturbation. We added a perturbation energy term $0.005 \cos(\omega t)(x_1 + x_2)$. Our stochastic simulations did find that the amplitude of the $\langle x_1 \rangle$ oscillation driven by the perturbation shows a maximum near that suggested by the absorption spectrum (see fig. 1(c)).

Discussion. – In this work, we derived some general FD relations for systems violating the detailed balance, and tested with some examples including a system showing limit cycle. We notice that some of the results or special cases of the results in this work have been derived previously, for example, eq. (6) and eq. (8). The novelty here is that we demonstrated a unified treatment for systems near equilibrium or nonequilibrium steady state, using a recently proved mapping between a general dynamic system described by Langevin equations relaxing to a steady state and a Hamiltonian system relaxing to the equilibrium state [23]. While many of the previous derivations of the general FD relations require special technical treatments, the derivation here, while general, parallels to the procedure in a standard equilibrium statistical physics textbook.

Further studies are needed for potential applications of the generalized FD relation on studying systems described by eq. (1) [12,37]. As an example, one can use it on biological network reconstruction. The matrix $M$ contains information on the network topology and parameter values. Researchers proposed to use the relaxation dynamics to derive information of a biological network, especially a linear network [38,39]. A potential problem is that the relaxation dynamics alone may contain insufficient information to resolve a network topology and parameters, and to distinguish competing models. The FD relation provides additional constraints, and may serve as a criterion for evaluating different models. It remains to be examined if one can distinguish abnormal (e.g., cancer) cells from normal cells based on their differences of relaxation and fluctuation dynamics.

We suggest that one should further exploit the analogy between the dissipative and Hamiltonian systems. Many existing results for the latter may lead to new understanding for the former, provided appropriate quantities can be identified. As an example, researchers have used oscillating signals to perturb biological systems. They found that the oscillation amplitude of the variable being driven shows a maximum at certain driving frequency [40,41]. Here we showed that this phenomenon can be interpreted as the van Vleck-Weisskopf-Fröhlich-type resonance absorption [30]. The analogy may suggest further technical development in biological network studies parallel to the linear and nonlinear spectral methods used in physics and chemistry. Study analogous to Onsager’s reciprocal relations is another example [5,6]. A potential difficulty is to relate the mapped quantities to physically measurable quantities.

The relaxation dynamics is important for characterizing the dynamics of a system. For example, the resistor

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model suggests that a HIV slows down its relaxation from an unstable active excited state to a stable dormant state through a series of intermediate steps in its regulation network [42]. Wang and coworkers found that many biological networks have rugged potential profiles (as defined by eq. (4)), which resemble what observed in protein folding studies [43–45]. The finding reinforces that dynamics of biological systems is complex. Implications of noises in biological systems have been extensively discussed [46]. Here the mapping relates noise intensity to an effective temperature. Consequently we suggest that noise prevents a system from trapping into large numbers of undesired intermediate steady states a complex system may have. Therefore, the counter-intuitively existence of proper amount of noises, together with funneled landscapes [43], enhances rather than destroying the robustness of a network. Glass transition is an active research topic for the relaxation process of a physical system to an equilibrium state [47–49]. A typical biological network is highly inhomogeneous, and is full of competing interactions. Thus, its dynamics in some sense resembles that of spin glasses but with nonrandom quenching [49]. It is interesting to notice that the mapping between a dissipative and Hamiltonian system suggests possible glassy behaviors for relaxation to a nonequilibrium steady state. If being identified (noticing that glassy state has been identified in protein folding studies [48,50], also refer to Chapt. 6 of ref. [49]) in a spin glass model in the form of eq. (1)), it may have profound practical implications. For example, a patient might then have prolonged recovery period to the normal homeostatic state after a disease. One solution is to increase the temperature (i.e., noise intensity in the related regulation network) above the critical glass transition temperature. Indeed cells can regulate their noise levels [51].

It is worth noticing that, for the last example, the results of Langevin equations are averaged over $5 \times 10^5$ trajectories. Rigorously speaking, there is a correction term to the Langevin equation. Our numerical algorithm adopts the Itô interpretation. In [23], we discussed the relation between the Itô interpretation and the zero-mass interpretation adopted for deriving the mapping Hamiltonian. The expression of the correction term can be derived straightforwardly. However, the correction term is proportional to $1/\beta$, and is small for this system. Therefore we neglected this term here.

In this work we only established a framework. Most of our discussions focus on biological examples. They equally apply to problems in other fields sharing the same mathematical structure, e.g., a stock market model described by eq. (1).

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