Local fluctuation-dissipation relations far from equilibrium

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Motivation

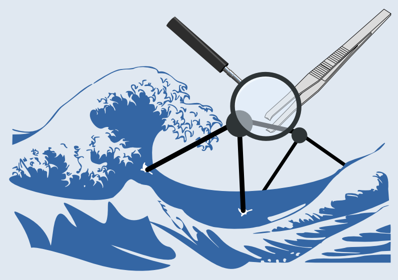
At equilibrium, where all thermodynamic currents vanish on average, the fluctuation-dissipation relation (FDR) connects the response $R^{\mathrm{eq}} := \frac{\partial J_\alpha}{\partial h_\alpha}\Big|_{h=0}$ of a current J to a conjugate field h with its fluctuations, which are characterized by the diffusion coefficient $D^{\mathrm{eq}} := D(\boldsymbol{h}=0)$:

$$D^{\mathrm{eq}} = TR^{\mathrm{eq}}$$

Often, only a subset of all currents can be observed, while others are hidden. A system where all observed currents stall (i.e. where they vanish on average), at first glance resembles an equilibrium system, although the presence of hidden currents may strongly influence the observed ones.

Research Question

Does an equilibrium-like FDR hold for a single current quietly stalling within an ocean of non-equilibrium?



Main result [1]

Under stalling conditions, $J_{\mathrm{loc}}(\boldsymbol{h}^\star)=0$, the response $R^\star := \frac{\partial J_{\mathrm{loc}}}{\partial h_{\mathrm{loc}}}\Big|_{\boldsymbol{h}=\boldsymbol{h}^\star}$ of a local current $J_{\mathrm{loc}}(\boldsymbol{h})$ to a conjugate local perturbation h_{loc}, obeys a nonequilibrium FDR that takes the equilibrium form:

$$D^\star = TR^\star$$

Dynamics

- Markov jump processes are random walks $\boldsymbol{\omega}$ on a graph, characterized by transitions along edges $\mathbf{e}_k$ at times t_k

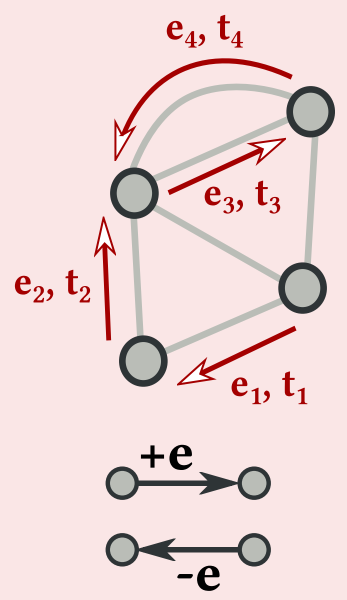
$$\boldsymbol{\omega} = (\omega_0 \xrightarrow{\mathrm{e}_1, t_1} \omega_1 \xrightarrow{\mathrm{e}_2, t_2} \dots)$$

- transition rates $w_{\mathrm{e}} = w_{\mathrm{e}}(\boldsymbol{h})$ depend on external parameters $\boldsymbol{h}=\{h_\alpha\}_\alpha$
- Master equation for probabilities $p_\omega^{(t)}$

$$p_\omega^{(t)} = \sum_{\omega'} \sum_{\mathrm{e}:\, \omega' \to \omega} J_{\mathrm{e}}^{(t)}$$

with instantaneous probability currents along edges $\mathbf{e}$: ω' ⟶ ω

$$J_{\mathrm{e}}^{(t)} = p_{\omega'}^{(t)} w_{\mathrm{e}} - p_\omega^{(t)} w_{-\mathrm{e}}$$



- stationary currents $J_{\mathrm{e}}^{(t)} \to J_{\mathrm{e}}$ balance at each vertex ω
- at equilibrium, all currents vanish: $J_{\mathrm{e}} = 0 \quad \forall \mathrm{e}$

Fluctuating Physical Currents [2]

- instantaneous fluctuating current for the transport of extensive physical quantity d^α

$$j_\alpha^{(t)}[\boldsymbol{\omega}] = \sum_{k=1}^{\infty} \delta(t - t_k) d^\alpha_{\mathrm{e}_k}$$

with thermodynamic distances $d^\alpha_{\mathrm{e}} = d^\alpha_{-\mathrm{e}}$

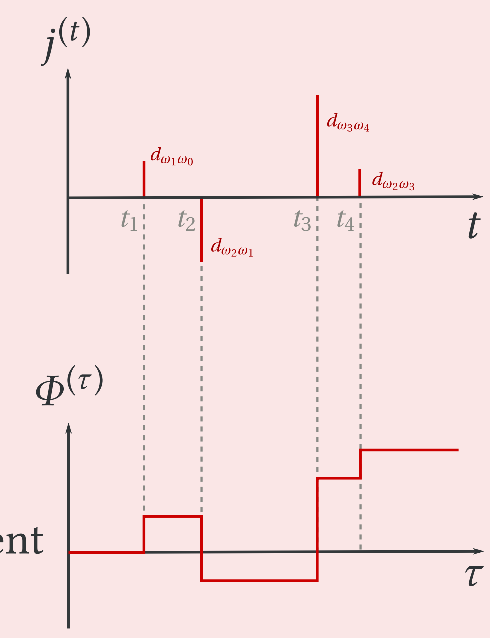
- time-integrated currents

$$\Phi_\alpha^{(\tau)}[\boldsymbol{\omega}] = \int_{t=0}^{\tau} \Phi_\alpha^{(t)}[\boldsymbol{\omega}]\, \mathrm{d}t = \sum_{k=1}^{n(\tau)} d^\alpha_{\mathrm{e}_k}$$

- time-averaged currents converge to stationary current

$$J_\alpha = \frac{1}{2} \sum_{\mathrm{e}} d^\alpha_{\mathrm{e}} J_{\mathrm{e}} = \lim_{\tau\to\infty} \frac{1}{\tau} \left\langle \Phi_\alpha^{(\tau)} \right\rangle_{\boldsymbol{h}}$$

where $\langle \cdot \rangle_{\boldsymbol{h}}$ denotes a trajectory average for given parameters $\boldsymbol{h}$



Motance, Sensitivities and Locality [1,5]

- motance (driving force) for edge $\mathbf{e}$: $\quad B_{\mathrm{e}} := \ln\left(\frac{w_{\mathrm{e}}}{w_{-\mathrm{e}}}\right)$
- α-sensitivity for edge $\mathbf{e}$: $\quad r^\alpha_{\mathrm{e}} := \partial_{h_\alpha} \ln(w_{\mathrm{e}})$
- $\mathbf{e}$-local α-perturbation: $\quad r^\alpha_{\mathrm{e}'} = 0 \quad \forall \mathrm{e}' \neq \pm\mathrm{e}$
- $\mathbf{e}$-local α-current: $\quad d^\alpha_{\mathrm{e}'} = 0 \quad \forall \mathrm{e}' \neq \pm\mathrm{e}$

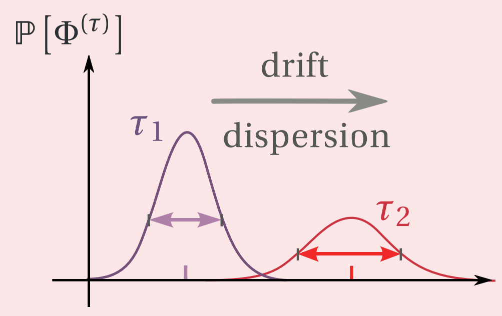
Response and Fluctuations [2,3]

- response coefficient

$$R_{\alpha\beta} = \frac{\partial J_\alpha}{\partial h_\beta}$$

- diffusion / dispersion / Green–Kubo integral

$$D_{\alpha\beta} = \lim_{\tau\to\infty} \frac{1}{2\tau} \left\langle \Phi_\alpha^{(\tau)} \Phi_\beta^{(\tau)} \right\rangle_{\boldsymbol{h}} = \int_0^\infty \left\langle (j_\alpha^{(0)} - J_\alpha)\, (j_\beta^{(t)} - J_\beta) \right\rangle_{\boldsymbol{h}} \mathrm{d}t$$



General Mathematical Result [1]

For an $\mathbf{e}$-local α-perturbation at stalling conditions $\boldsymbol{h}^\star$ such that $J_{\mathrm{e}}(\boldsymbol{h}^\star)=0$, it holds that

$$\frac{\partial J_{\mathrm{e}}}{\partial h_\alpha}\bigg|_{\boldsymbol{h}^\star} = \frac{\partial B_{\mathrm{e}}}{\partial h_\alpha}\bigg|_{\boldsymbol{h}^\star} \int_0^\infty \left\langle j_{\mathrm{e}}^{(0)}\, j_{\mathrm{e}}^{(t)} \right\rangle_{\boldsymbol{h}^\star} \mathrm{d}t$$

The proof [1] uses the determinant structure of the tilted generator, known from the theory of large deviations [3,4].

Local Detailed Balance [5]

Local detailed balance (LDB) ensures conjugacy between physical currents $J_\alpha(\boldsymbol{h})$ and external fields h_α

$$B_{\mathrm{e}} \stackrel{!}{=} \frac{1}{T} \sum_\alpha h_\alpha d^\alpha_{\mathrm{e}} \quad \Leftrightarrow \quad T\frac{\partial B_{\mathrm{e}}}{\partial h_\alpha} \equiv T(r^\alpha_{\mathrm{e}} - r^\alpha_{-\mathrm{e}}) \stackrel{!}{=} d^\alpha_{\mathrm{e}}$$

Thermodynamic Result [1]

Under the assumption of local detailed balance, the response of a stalled local physical current $J_\alpha(\boldsymbol{h}) = d^\alpha_{\mathrm{e}} J_{\mathrm{e}}(\boldsymbol{h})$ along a single edge $\mathbf{e}$ to an $\mathbf{e}$-local conjugate perturbation h_α obeys the equilibrium-like FDR

$$TR_{\alpha\alpha}(\boldsymbol{h}^\star) \equiv \frac{\partial J_\alpha}{\partial h_\alpha}\bigg|_{\boldsymbol{h}^\star} = \int_0^\infty \left\langle j_\alpha^{(0)}\, j_\alpha^{(t)} \right\rangle_{\boldsymbol{h}^\star} \mathrm{d}t = D(\boldsymbol{h}^\star)$$

Summary and Outlook

Fluctuating currents generated by **Markov jump processes** are the central concept in Stochastic Thermodynamics. Here, we discussed the connection between the response of a local stalled current to a local perturbation and its fluctuations. For physical models obeying **local detailed balance**, a general **mathematical result** implies our **main physical result**, namely the validity of a nonequilibrium fluctuation-dissipation relation (FDR) in the well-known equilibrium form.

Future work seeks to generalize the conditions for the validity of equilibrium-like FDRs in situations far from equilibrium.

References

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[4] H Touchette, Phys Rep 478, 1 (2009)
[5] U Seifert, Phys Rev Lett 104, 138101 (2010)