Stochastic Thermodynamics and Thermodynamics of Information

Lecture III: Systems without Detailed Balance

Luca Peliti

May 4, 2018

Statistical Physics, SISSA and SMRI (Italy)

Table of contents

Recapitulation

- Master equation:

$$\frac{\mathrm{d}p_x}{\mathrm{d}t} = \sum_{x'\,(\neq x)}{}' \left[R_{xx'}(\lambda)p_{x'} - R_{x'x}(\lambda)p_x\right] = (\mathcal{L}_\lambda\, p)_x$$

- Detailed-balance (DB) condition:

$$R_{xx'}\mathrm{e}^{(F-E_{x'})/k_\mathrm{B}T} = R_{x'x}\mathrm{e}^{(F-E_x)/k_\mathrm{B}T}$$

- Properties of the rates:

$$\frac{R_{x'x}}{R_{xx'}} = \mathrm{e}^{-Q_{x'x}/k_\mathrm{B}T} = \mathrm{e}^{\Delta S^{(\mathrm{r})}/k_\mathrm{B}}$$

- Seifert's identity:

$$\frac{\mathcal{P}_{\boldsymbol{\lambda}}(\boldsymbol{x})}{\mathcal{P}_{\hat{\boldsymbol{\lambda}}}(\hat{\boldsymbol{x}})} = \mathrm{e}^{(\Delta S^{(\mathrm{r})}(\boldsymbol{x})+\Delta s)/k_\mathrm{B}} = \mathrm{e}^{\Delta_\mathrm{i} S(\boldsymbol{x})/k_\mathrm{B}}$$

- Jarzynski's equality:

$$\underbrace{\left\langle \mathrm{e}^{-\mathcal{W}/k_\mathrm{B}T} \right\rangle}_{\text{non-eq.}} = \underbrace{\mathrm{e}^{-\Delta F/k_\mathrm{B}T}}_{\text{eq}}$$

Fluctuation-Response relation

Linear response:

- Perturbation of a DB system:

$$E_x(\lambda) = E_x^{(0)} - \sum_\alpha \lambda_\alpha A_x^\alpha$$

- Unperturbed distribution: $p_x^{(0)} = \mathrm{e}^{(F^{(0)} - E_x^{(0)})/k_\mathrm{B}T}$

$$\langle A^\alpha \rangle^{(0)} = \sum_x A_x^\alpha \, p_x^{(0)}$$

- Manipulation protocol: $\boldsymbol{\lambda} = (\lambda(t))$, $\lambda(t)$ small, $\forall t$, $\lambda(t) = 0$, $t < 0$
- Perturbed averages: define $\delta A_x^\alpha = A_x^\alpha - \langle A^\alpha \rangle^{(0)}$

$$\langle \delta A^\alpha \rangle_{p(t)} = \sum_x \delta A_x^\alpha \, p_x(t) \simeq \sum_\beta \int_0^t \mathrm{d}t' \; \chi_{\alpha\beta}(t - t') \, \lambda_\beta(t')$$

- $\chi_{\alpha\beta}(t - t') = 0$ for $t' > t$ (causality)

Fluctuation-Response relation

Correlation functions:

- $C_{\alpha\beta}(t-t') = \sum_{xx'} \delta A^\alpha_x \, \delta A^\beta_{x'} \, P^{(0)}(x,t;x',t')$
- $P^{(0)}(x,t;x',t') = \left(\exp\left((t-t')\mathcal{L}_0\right)\right)_{xx'} p^{(0)}_{x'}$
- $C_{\alpha\beta}(t-t') = C_{\alpha\beta}(t'-t)$ (assuming A^α to be time-inversion invariant) (exercise!)
- $C_{\alpha\beta}(0) = \left\langle \delta A^\alpha \, \delta A^\beta \right\rangle^{(0)}$
- $\lim_{t\to\infty} C_{\alpha\beta}(t-t') = 0$

Fluctuation-Response relation:

$$\boxed{\chi_{\alpha\beta}(t) = -\frac{\theta(t)}{k_\mathrm{B}T}\frac{\mathrm{d}}{\mathrm{d}t} C_{\alpha\beta}(t)}$$

Fluctuation-Response relation

Proof:

- Let $\lambda_\alpha(t) = \lambda_\alpha\, \delta(t-t')$, then $\langle \delta A^\alpha \rangle_{p(t)} = \sum_\beta \chi_{\alpha\beta}(t-t')\, \lambda_\beta$
- Therefore

$$\lim_{t\to t'+} p(t) = p^* = p^{(0)} + \sum_\alpha \lambda_\alpha \frac{\partial \mathcal{L}_\lambda}{\partial \lambda_\alpha} p^{(0)}$$

$$p(t) = \exp\big((t-t')\mathcal{L}_0\big)\, p^*$$

- "Perturbed" equilibrium distribution $\mathcal{L}_\lambda p^{(\lambda)} = 0$:

$$p_x^{(\lambda)} = \mathrm{e}^{(F_\lambda - E_x^{(0)} + \sum_\alpha \lambda_\alpha A_x^\alpha)/k_\mathrm{B}T}$$

Thus

$$\left.\frac{\partial \mathcal{L}_\lambda}{\partial \lambda_\alpha}\right|_{\lambda=0} p^{(0)} + \mathcal{L}_0 \left.\frac{\partial p^{(\lambda)}}{\partial \lambda_\alpha}\right|_{\lambda=0} = 0$$

which implies

$$\left.\frac{\partial \mathcal{L}_\lambda}{\partial \lambda_\alpha}\right|_{\lambda=0} p^{(0)} = -\mathcal{L}_0 \left.\frac{\partial \log p^{(\lambda)}}{\partial \lambda_\alpha}\right|_{\lambda=0} p^{(0)} = -\frac{1}{k_\mathrm{B}T}\mathcal{L}_0 \left(A^\alpha - \langle A^\alpha \rangle^{(0)}\right) p^{(0)}$$

Fluctuation-Response relation

- Thus, for $t > t'$,

$$\chi_{\alpha\beta}(t-t') = -\frac{1}{k_{\mathrm{B}}T}\sum_{x'x}\delta A^{\alpha}_{x'}\left[\exp\left((t-t')\mathcal{L}_0\right)\mathcal{L}_0\right]_{x'x}\delta A^{\beta}_{x}\,p^{(0)}_{x}$$
$$= \frac{1}{k_{\mathrm{B}}T}\frac{\partial}{\partial t'}C_{\alpha\beta}(t-t') = -\frac{1}{k_{\mathrm{B}}T}\frac{\partial}{\partial t}C_{\alpha\beta}(t-t')$$

Therefore, $\forall t$,

$$\frac{1}{k_{\mathrm{B}}T}\frac{\mathrm{d}}{\mathrm{d}t}C_{\alpha\beta}(t) = \chi_{\alpha\beta}(-t) - \chi_{\alpha\beta}(t)$$

and by taking the Fourier transform, the fluctuation-response relation

$$\boxed{\mathrm{Im}\,\tilde{\chi}_{\alpha\beta}(\omega) = \frac{\omega\,\tilde{C}_{\alpha\beta}(\omega)}{2k_{\mathrm{B}}T}}$$

Non-equilibrium steady states (NESS)

DB requires that $\forall x, y, z$ one has

$$R_{xy}R_{yz}R_{zx} = R_{zy}R_{yx}R_{xz}$$

If this does not obtain, $\nexists E_x : \quad R_{x'x}/R_{xx'} = \mathrm{e}^{-(E_{x'}-E_x)/k_\mathrm{B}T}$

One can still quite generally have p^ss satisfying

$$\sum_{x'} R_{xx'}p^\mathrm{ss}_{x'} = \sum_{x'} R_{x'x}p^\mathrm{ss}_x$$

Assume that the transition is helped by one (or more!) reservoir:

$$\Delta S^{(\mathrm{r})}_{xx'} = k_\mathrm{B}\log\frac{R_{xx'}}{R_{x'x}}$$

Then

$$\frac{\mathcal{P}(\boldsymbol{x}|x(0))}{\mathcal{P}(\hat{\boldsymbol{x}}|\hat{x}(0))} = \prod_{t=0}^{t_\mathrm{f}-1}\frac{R_{x(t+1)x(t)}}{R_{x(t)x(t+1)}} = \mathrm{e}^{\Delta S^{(\mathrm{r})}(\boldsymbol{x})/k_\mathrm{B}}$$

Fluctuation theorem

Choose $p_x(t_0) = p_x(t_\mathrm{f}) = p_x^\mathrm{ss}$

$$\log \frac{\mathcal{P}(\boldsymbol{x})}{\mathcal{P}(\hat{\boldsymbol{x}})} = \left(\Delta S^{(\mathrm{r})}(\boldsymbol{x}) + \Delta S^{\mathcal{S}}\right)/k_\mathrm{B}$$

Total entropy production:

$$\Delta S^\mathrm{tot} = \Delta S^{(\mathrm{r})}(\boldsymbol{x}) + \Delta S$$

Summing over all paths $\boldsymbol{x}$ with a given value of ΔS^tot yields the fluctuation theorem:

$$\boxed{\frac{p(\Delta S^\mathrm{tot})}{p(-\Delta S^\mathrm{tot})} = \mathrm{e}^{\Delta S^\mathrm{tot}/k_\mathrm{B}}}$$

Evans-Searles, 1994, Gallavotti and Cohen, 1995-6

Comment

- The fluctuation theorem holds for *finite times*, starting from the steady state
- Since ΔS is bounded, but $\Delta S^{(\mathrm{r})}$ grows, we have for large t_{f}

$$\Delta S^{\mathrm{tot}} \simeq \Delta S^{(\mathrm{r})}$$

- Large-deviation function $\phi(s)$:

$$p(\Delta S^{\mathrm{tot}}) \propto \mathrm{e}^{-t_{\mathrm{f}}\phi(\Delta S^{\mathrm{tot}}/(k_{\mathrm{B}}t_{\mathrm{f}}))}$$

  Gallavotti-Cohen relation:

$$\boxed{\phi(s) = \phi(-s) - s}$$

- Generating function:

$$\psi(\mu) = -\frac{1}{t_{\mathrm{f}}} \log \int \mathrm{d}s\ \mathrm{e}^{-t_{\mathrm{f}}(\phi(s)+\mu s)}$$

$$s^*(\mu) : \phi'(s^*) = -\mu \qquad \psi(\mu) = \phi(s^*) + \mu\, s^*$$

- Symmetry relation: (Lebowitz and Spohn, 1999)

$$\boxed{\psi(\mu) = \psi(1-\mu)}$$

Equation for the generating function

- Define

$$\Psi_x(\mu, t) = \int \mathcal{D}\boldsymbol{x}\; \mathcal{P}^{\rm ss}(\boldsymbol{x})\, \delta_{x(t)x}\, \mathrm{e}^{-\mu S^{\rm tot}(\boldsymbol{x})/k_{\rm B}}$$

- Then

$$\frac{\partial \Psi_x}{\partial t} = \sum_{x'\,(\neq x)}{}' \left[R_{xx'} \left(\frac{R_{x'x}}{R_{xx'}} \right)^{\mu} \Psi_{x'} - R_{x'x} \Psi_x \right] = \left(\mathcal{L}^{\rm LS}_{\mu}\, \Psi \right)_x$$

- Now

$$\mathcal{L}^{\rm LS}_{\mu} = \mathcal{L}^{\rm LS}_{1-\mu}{}^{\dagger}$$

- Thus $\mathcal{L}^{\rm LS}_{1-\mu}$ and $\mathcal{L}^{\rm LS}_{\mu}$ have the same spectrum
- But

$$\Psi_x(t) = \left(\exp\left(t \mathcal{L}^{\rm LS}_{\mu} \right)\, \Psi(0) \right)_x \sim \exp\left(t\, \Lambda^{\rm LS}_{\max}(\mu) \right)$$

- We have

$$\psi(\mu) = -\log \Lambda^{\rm LS}_{\max}(\mu) = -\log \Lambda^{\rm LS}_{\max}(1-\mu) = \psi(1-\mu)$$

Housekeeping entropy production

Stationary system:

$$\Delta S_{x'x}/k_{\mathrm{B}} = \log \frac{R_{x'x}}{R_{xx'}}$$
$$= \underbrace{\log \frac{R_{x'x} p_x^{\mathrm{ss}}}{R_{xx'} p_{x'}^{\mathrm{ss}}}}_{\Delta \mathcal{S}^{(\mathrm{hk})}/k_{\mathrm{B}}} - \underbrace{\log \frac{p_x^{\mathrm{ss}}}{p_{x'}^{\mathrm{ss}}}}_{\Delta S^{(\mathrm{ex})}/k_{\mathrm{B}}}$$

N.B.: If detailed balance is satisfied:

$$R_{xx'} p_{x'}^{\mathrm{ss}} = R_{x'x} p_x^{\mathrm{ss}}$$

then

$$\Delta S_{x'x}^{(\mathrm{hk})} = 0 \qquad \forall x, x'$$

Non-stationary system

Rewrite this section including Hatano-Sasa

$$\Delta S^{(\mathrm{r})}_{xx'}/k_\mathrm{B} = \log \frac{R_{xx'}}{R_{x'x}} = \underbrace{\log \frac{R_{xx'}p_{x'}}{R_{x'x}p_x}}_{\Delta S^{\mathrm{tot}}_{xx'}/k_\mathrm{B}} \underbrace{- \log \frac{p_{x'}}{p_x}}_{-\Delta S_{xx'}/k_\mathrm{B}}$$

$$\left\langle \dot{S}^{\mathrm{tot}} \right\rangle = \frac{k_\mathrm{B}}{2} \sum_{xx'} \underbrace{\left(R_{xx'}p_{x'} - R_{x'x}p_x\right)}_{J_{xx'}} \underbrace{\log \frac{R_{xx'}p_{x'}}{R_{x'x}p_x}}_{X_{xx'}}$$

$$X_{xx'} = \underbrace{\log \frac{R_{xx'}p^{\mathrm{ss}}_{x'}}{R_{x'x}p^{\mathrm{ss}}_{x}}}_{X^{(\mathrm{hk}\,(\mathrm{ad.}))}_{xx'}} + \underbrace{\log \frac{p_{x'}p^{\mathrm{ss}}_{x}}{p_x p^{\mathrm{ss}}_{x'}}}_{X^{(\mathrm{n.ad.})}_{xx'}}$$

$$\left\langle \dot{S}^{\mathrm{tot}} \right\rangle = \underbrace{\frac{k_\mathrm{B}}{2} \sum_{xx'} J_{xx'} X^{(\mathrm{ad.})}_{xx'}}_{\left\langle \dot{S}^{(\mathrm{hk})} \right\rangle \geq 0} + \underbrace{\frac{1}{2} \sum_{xx'} J_{xx'} X^{(\mathrm{n.ad.})}_{xx'}}_{\left\langle \dot{S}^{(\mathrm{n.ad.})} \right\rangle \geq 0}$$

Average housekeeping heat

$$\left\langle \dot{S}^{(\mathrm{hk})} \right\rangle = k_{\mathrm{B}} \sum_{x'\,(\neq x)}{}' \sum_{x} R_{x'x} \log \frac{R_{x'x} p^{\mathrm{ss}}_{x}}{R_{xx'} p^{\mathrm{ss}}_{x'}}$$

$$= k_{\mathrm{B}} \sum_{x<x'}{}' \left(R_{x'x} p^{\mathrm{ss}}_{x} - R_{xx'} p^{\mathrm{ss}}_{x'}\right) \log \frac{R_{x'x} p^{\mathrm{ss}}_{x}}{R_{xx'} p^{\mathrm{ss}}_{x'}} \geq 0$$

We also have

$$\mathcal{P}^{\mathrm{ss}}(\boldsymbol{x})\, \mathrm{e}^{-\Delta S^{(\mathrm{hk})}(\boldsymbol{x})/k_{\mathrm{B}}} = \mathcal{P}^{\mathrm{ss}}(\hat{\boldsymbol{x}}) \prod_{k=1}^{n} \frac{p^{\mathrm{ss}}_{x_k}}{p^{\mathrm{ss}}_{x_{k-1}}} \left(\frac{p^{\mathrm{ss}}_{x_0}}{p^{\mathrm{ss}}_{x_n}} \right)$$

which implies the integral fluctuation theorem

$$\left\langle \mathrm{e}^{-\Delta S^{(\mathrm{hk})}/k_{\mathrm{B}}} \right\rangle = 1$$

One also has

$$\left\langle \mathrm{e}^{-\Delta S^{(\mathrm{n.ad})}/k_{\mathrm{B}}} \right\rangle = 1$$

Parameter-dependent steady state:

$$R_{x'x}(\lambda) \longrightarrow p_x^{\mathrm{ss}}(\lambda)$$

$$(\mathcal{L}_\lambda\, p^{\mathrm{ss}}(\lambda))_x = \sum_{x'\,(\neq x)}{}' \left[R_{xx'}(\lambda)p_{x'}^{\mathrm{ss}}(\lambda) - R_{x'x}(\lambda)p_x^{\mathrm{ss}}(\lambda)\right] = 0$$

$$\Delta S^{\mathrm{ex}} = \Delta S^{\mathrm{tot}} - \Delta S^{(\mathrm{hk})}$$

Manipulating the steady state:

$$\boldsymbol{\lambda} = \lambda(t) \qquad \lambda(0) = \lambda_0 \qquad \lambda(t_{\mathrm{f}}) = \lambda_{\mathrm{f}}$$

$$\mathcal{P}_{\boldsymbol{\lambda}}(\boldsymbol{x}) = \mathcal{P}_{\boldsymbol{\lambda}}(\boldsymbol{x}|x(0))p_x^{\mathrm{ss}}(\lambda_0)$$

The excess entropy production

$$\phi_x(\lambda) = -\log p^{\mathrm{ss}}(x,\lambda)$$
$$\Delta S^{(\mathrm{ex})}_{x'x}(\lambda) = -\left(\phi_{x'}(\lambda) - \phi_x(\lambda)\right)$$

$$\begin{aligned}
\Delta S^{(\mathrm{ex})}(\boldsymbol{x}) &= \sum_{k=1}^{n} \Delta S^{(\mathrm{ex})}_{x_k x_{k-1}}(\lambda(t_k)) \\
&= -\sum_{k=1}^{n} \left[\phi_{x_k}(\lambda(t_k)) - \phi_{x_{k-1}}(\lambda(t_k))\right] \\
&= -\phi_{x_\mathrm{f}}(\lambda(t_\mathrm{f})) + \underbrace{\sum_{k=0}^{n} \left[\phi_{x_k}(\lambda(t_{k+1})) - \phi_{x_k}(\lambda(t_k))\right]}_{\mathcal{A}(\boldsymbol{x})} + \phi_{x_0}(\lambda(t_0)) \\
&= -\Delta\phi + \mathcal{A}(\boldsymbol{x})
\end{aligned}$$

$$\mathcal{A}(t_\mathrm{f}, \boldsymbol{x}) = \sum_{k=0}^{n} \left[\phi_{x_k}(\lambda(t_{k+1})) - \phi_{x_k}(\lambda(t_k))\right] = \int_{t_0}^{t_\mathrm{f}} \mathrm{d}t\ \dot{\lambda}(t)\, \partial_\lambda \phi_{x(t)}(\lambda(t))$$

The Hatano-Sasa relation

Hatano and Sasa, 2001

Relation analogous to Jarzynski's for manipulated steady states out of equilibrium

- Manipulate λ: $\boldsymbol{\lambda} = (\lambda(t))$, $t \in [t_0, t_{\mathrm{f}}]$
- Initial condition:

$$p_x(t_0) = p_x^{\mathrm{ss}}(\lambda_0)$$

- Then

$$\left\langle \mathrm{e}^{-\mathcal{A}} \right\rangle = 1$$

Proof

Define

$$\Psi_x(t) = \int \mathcal{D}\boldsymbol{x}\ \delta_{x(t),x}\, \mathrm{e}^{-\mathcal{A}(t,\boldsymbol{x})}\, \mathcal{P}(\boldsymbol{x})$$

Then

$$\Psi_x(t_0) = p_x^{\mathrm{ss}}(\lambda_0)$$

$$(\mathcal{L}_\lambda)_{xx'} = R_{xx'}(\lambda) - \sum_y R_{yx}\ \delta_{xx'}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\Psi_x(t) = \left(\mathcal{L}_{\lambda(t)}\Psi\right)_x - \dot{\lambda}\partial_\lambda \phi_x(\lambda(t))\,\Psi_x(t)$$

Ansatz:

$$\Psi_x(t) = \mathrm{e}^{-\phi_x(\lambda(t))} = p_x^{\mathrm{ss}}(\lambda(t))$$

Then

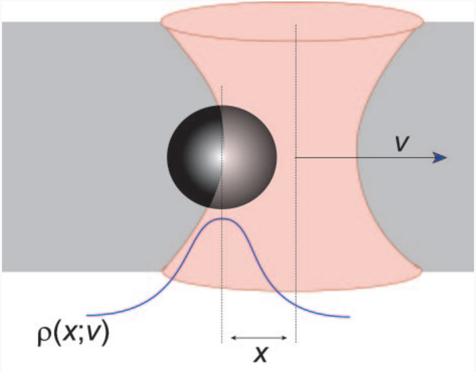
$$\frac{\mathrm{d}}{\mathrm{d}t}\Psi_x(t) = \underbrace{\left(\mathcal{L}_{\lambda(t)} p^{\mathrm{ss}}(\lambda(t))\right)_x}_{=0} - \dot{\lambda}\partial_\lambda \phi_x(\lambda(t))\,\mathrm{e}^{-\phi_x(\lambda(t))}$$

$$\left\langle \mathrm{e}^{-\mathcal{A}} \right\rangle = \sum_x \Psi_x(t) = \sum_x p_x^{\mathrm{ss}}(\lambda(t)) = 1$$

Experimental test of the Hatano-Sasa relation

TREPAGNIER ET AL., 2004

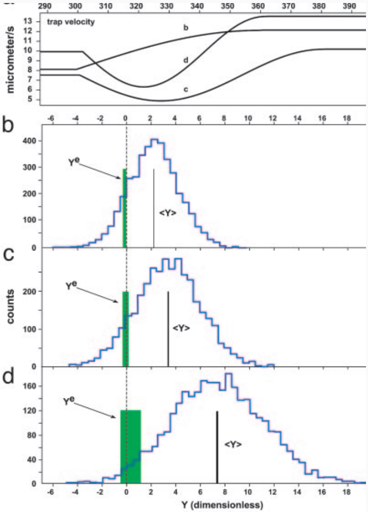
A Brownian colloidal particle dragged at constant speed by an optical tweezer



$$p^{\mathrm{ss}}(x;v) \propto \exp[-(\kappa x + \gamma v)^2/(2\kappa\, k_{\mathrm{B}} T)]$$

Experimental test of the Hatano-Sasa relation

Trepagnier et al., 2004



Characterizing active systems

- In a system at equilibrium at temperature T one has the Fluctuation-Response relation

$$\mathrm{Im}\,\tilde{\chi}(\omega) = \frac{\omega\,\tilde{C}(\omega)}{2k_{\mathrm{B}}T}$$

- In an active system there is a non-vanishing entropy-production rate, given on average by

$$\dot{S}^{\mathrm{tot}} = \frac{1}{2}\sum_{x\neq x'} J_{x'x}\log\frac{R_{x'x}}{R_{xx'}}$$

- We thus have two possible strategies for checking if a system is active:
    1. By checking the Fluctuation-Response relation (which requires measuring the response)
    2. By evaluating the entropy production

Non-equilibrium FR relation

PROST ET AL., 2009

- Small variations $\delta\lambda$ of the control parameter around $\lambda^{(0)}$
- Up to 2nd order in $\delta\lambda$

$$\langle \partial_{\lambda_\alpha}\phi(t_\mathrm{f})\rangle = \sum_\beta \int_{t_0}^{t_\mathrm{f}} \mathrm{d}t\ \delta\dot{\lambda}_\beta(t) \left\langle \partial_{\lambda_\alpha}\phi(t_\mathrm{f})\, \partial_{\lambda_\beta}\phi(t)\right\rangle$$

- But

$$\langle \partial_{\lambda_\alpha}\phi(t_\mathrm{f})\rangle \simeq \left\langle \partial_{\lambda_\alpha}\phi(\lambda^{(0)})\right\rangle + \sum_\beta \left\langle \partial_{\lambda_\alpha}\partial_{\lambda_\beta}\phi(\lambda^{(0)})\right\rangle\ \delta\lambda_\beta(t_\mathrm{f})$$

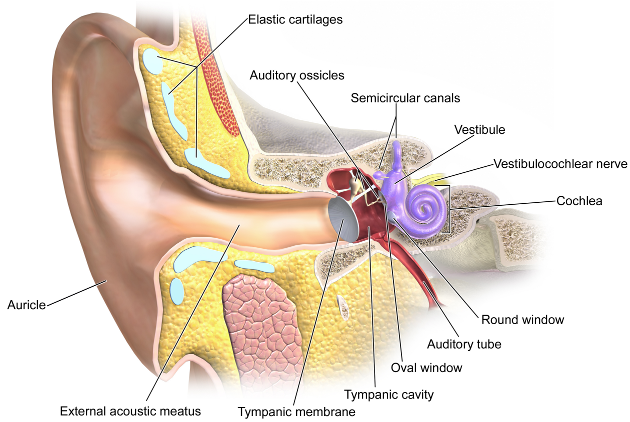
- Integrating by parts one obtains the FR relation:

$$\langle \partial_{\lambda_\alpha}\phi(t_\mathrm{f})\rangle = \sum_\beta \int_{t_0}^{t_\mathrm{f}} \mathrm{d}t'\ \chi_{\alpha\beta}(t_\mathrm{f}-t')\,\delta\lambda_\beta(t')$$

with

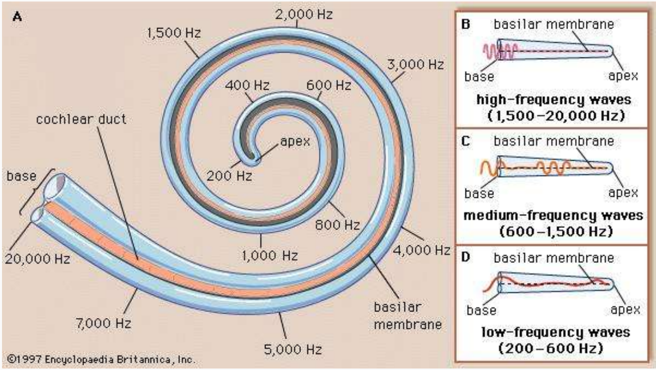
$$\chi_{\alpha\beta}(t-t') = \frac{\mathrm{d}}{\mathrm{d}t}\left\langle \partial_{\lambda_\alpha}\phi_{x(t)}(\lambda^{(0)})\,\partial_{\lambda_\beta}\phi_{x(t')}(\lambda^{(0)})\right\rangle$$

The Hair-Cell bundles

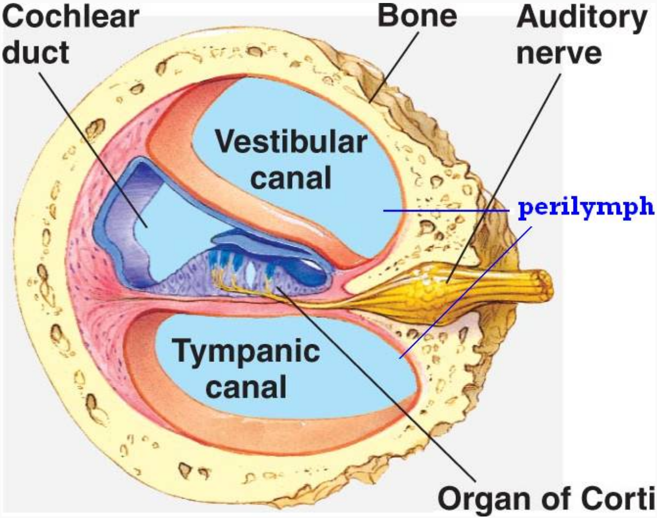


The Anatomy of the Ear

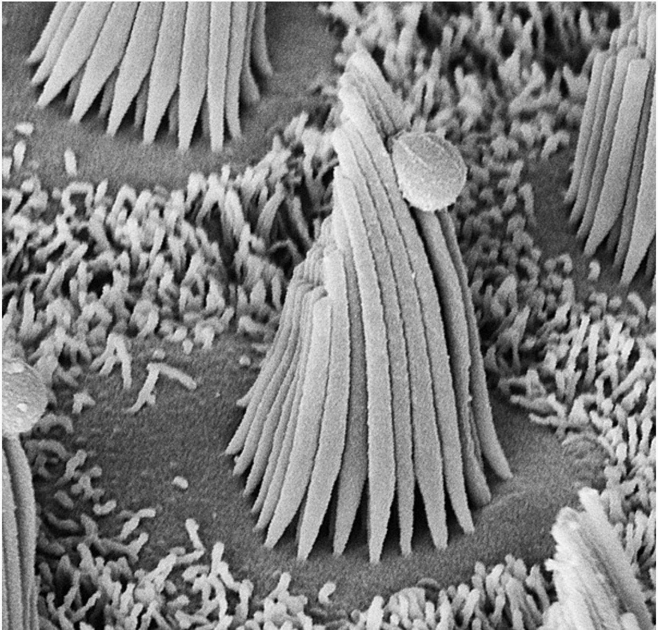
The Hair-Cell bundles



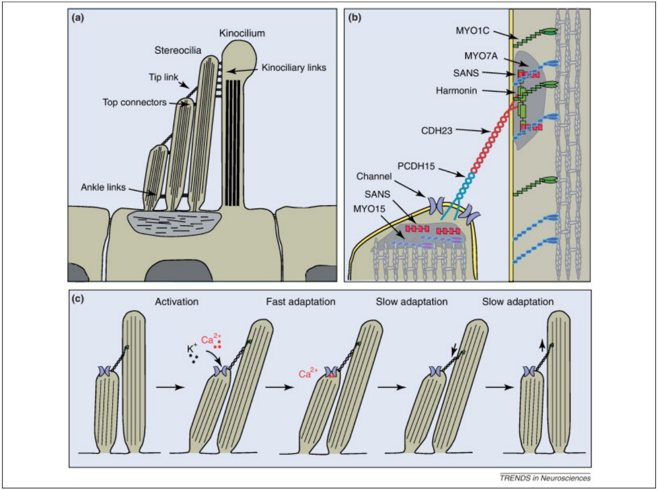
The Hair-Cell bundles



The Hair-Cell bundles



The Hair-Cell bundles



Non-equilibrium FR relation in the Hair-Cell bundle

DINIS ET AL., 2012

Dynamical system: x: hair-bundle deflection, y: force due to active process, ω_0: spontaneous oscillation frequency

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{pmatrix} x \\ y \end{pmatrix} = \underbrace{\begin{pmatrix} -r & \omega_0 \\ -\omega_0 & -r \end{pmatrix}}_{A} \begin{pmatrix} x \\ y \end{pmatrix} + \begin{pmatrix} f_x \\ 0 \end{pmatrix} + \begin{pmatrix} \eta_x \\ \eta_y \end{pmatrix}$$

Conjugate variables (X, Y):

$$\begin{pmatrix} X \\ Y \end{pmatrix} = \left(A^{-1}\right)^{\mathsf{T}} \underbrace{\Sigma_A^{-1}}_{\text{ss correlation}} \begin{pmatrix} x \\ y \end{pmatrix}$$

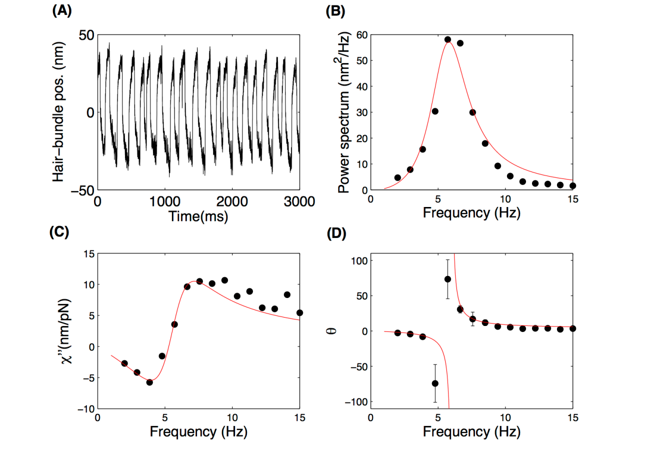
y is not directly observable...

Recast dynamics in terms of x and $z = y\omega_0 - rx$ such that when $f_x = 0$

$$\frac{\mathrm{d}x}{\mathrm{d}t} = z + \eta_x$$

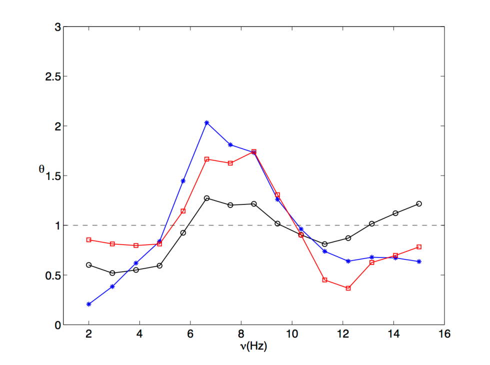
Non-equilibrium FR relation in the Hair-Cell bundle

Dinis et al., 2012



Non-equilibrium FR relation in the Hair-Cell bundle

Dinis et al., 2012



- Black: denoising of z
- Red: estimation of $\tilde{C}_{xz}(\omega)$
- Blue: estimation of y by max prob

$$\theta = \frac{\omega \tilde{C}_{XX}(\omega)}{2\tilde{\chi}''_{XX}(\omega)} = 1$$

Entropy production in the steady state

- Total entropy production:

$$\Delta S^{\mathrm{tot}} = \Delta S^{(\mathrm{r})} + \Delta S$$

- By Gallavotti-Cohen, Seifert etc.:

$$\Delta S^{\mathrm{tot}} = -\int \mathcal{D}\boldsymbol{x} \ \left[\frac{\mathcal{Q}(\boldsymbol{x})}{T} + k_{\mathrm{B}} \left(\log p^{\mathrm{ss}}_{x(\mathcal{T})} - \log p^{\mathrm{ss}}_{x(0)} \right) \right] \mathcal{P}^{\mathrm{ss}}(\boldsymbol{x}),$$

- Thus

$$\frac{\mathcal{P}^{\mathrm{ss}}(\boldsymbol{x})}{\mathcal{P}^{\mathrm{ss}}(\hat{\boldsymbol{x}})} = \mathrm{e}^{-(\mathcal{Q}(\boldsymbol{x})/k_{\mathrm{B}}T + \log p^{\mathrm{ss}}_{x_{\mathrm{f}}} - \log p^{\mathrm{ss}}_{x_0})} = \mathrm{e}^{\Delta S^{\mathrm{tot}}(\boldsymbol{x})},$$

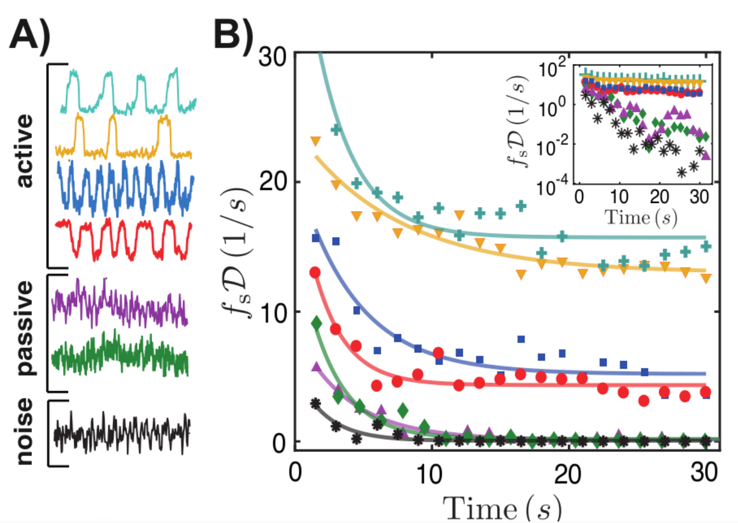
- Therefore

$$\Delta S^{\mathrm{tot}} = k_{\mathrm{B}} \int \mathcal{D}\boldsymbol{x} \ \mathcal{P}^{\mathrm{ss}}(\boldsymbol{x}) \log \frac{\mathcal{P}^{\mathrm{ss}}(\boldsymbol{x})}{\mathcal{P}^{\mathrm{ss}}(\hat{\boldsymbol{x}})} = k_{\mathrm{B}} D_{\mathrm{KL}}(\mathcal{P}^{\mathrm{ss}}(\boldsymbol{x}) \| \mathcal{P}^{\mathrm{ss}}(\hat{\boldsymbol{x}}))$$

Statistics on $\mathcal{P}^{\mathrm{ss}}(\boldsymbol{x})$ is hard to obtain...

Arrow of time in the Hair-Cell bundle

Roldán et al., 2018



Summary

- Fluctuation relations in systems without DB
- Generalization of link dissipation-irreversibility
- Generalization of FR relations
- Generalization to manipulated NESS

Questions:

- When do we decide if a system is active?
- What about feedback? (Demons!)

Thank you!

L. Dinis, P. Martin, J. Barral, J. Prost, and J. Joanny.
Fluctuation-response theorem for the active noisy oscillator of the hair-cell bundle.
Physical Review Letters, 109(16):160602, 2012.

D. J. Evans, E. Cohen, and G. Morriss.
Probability of second law violations in shearing steady states.
Physical Review Letters, 71:2401–2404, 1993.

D. J. Evans and D. J. Searles.
Equilibrium microstates which generate second law violating steady states.
Physical Review E, 50:1645–1648, 1994.

G. Gallavotti and E. G. D. Cohen.
Dynamical ensembles in nonequilibrium statistical mechanics.
Physical Review Letters, 74:2694–2697, 1995.

G. Gallavotti and E. G. D. Cohen.
Dynamical ensembles in stationary states.
Journal of Statistical Physics, 80:931–970, 1995.

J. Kurchan.
Fluctuation theorem for stochastic dynamics.
Journal of Physics A: Mathematical and General, 31(16):3719, 1998.

J. Kurchan.
Six out of equilibrium lectures.
arXiv preprint arXiv:0901.1271, 2009.

J. L. Lebowitz and H. Spohn.
A Gallavotti-Cohen-type symmetry in the large deviation functional for stochastic dynamics.
Journal of Statistical Physics, 95(1):333–365, 1999.

H. Oberhofer, C. Dellago, and P. L. Geissler.
Biased sampling of nonequilibrium trajectories: Can fast switching simulations outperform conventional free energy calculation methods?
The Journal of Physical Chemistry B, 109(14):6902–6915, 2005.

J. Prost, J.-F. Joanny, and J. M. R. Parrondo.
Generalized fluctuation-dissipation theorem for steady-state systems.
Physical Review Letters, 103:090601, Aug 2009.

É. Roldán.
Irreversibility and dissipation in microscopic systems.
Springer, 2014.

S. X. Sun.
Equilibrium free energies from path sampling of nonequilibrium trajectories.
The Journal of Chemical Physics, 118(13):5769–5775, 2003.

E. Trepagnier, C. Jarzynski, F. Ritort, G. E. Crooks, C. Bustamante, and J. Liphardt.
Experimental test of Hatano and Sasa's nonequilibrium steady-state equality.
Proceedings of the National Academy of Sciences of the United States of America, 101(42):15038–15041, 2004.

Édgar Roldán, J. Barral, P. Martin, J. M. R. Parrondo, and F. Jülicher.
Arrow of time in active fluctuations.
arXiv:1803:04743, 2018.