Large Deviations in Periodically Driven Systems

Optimally coarse-graining current fluctuations

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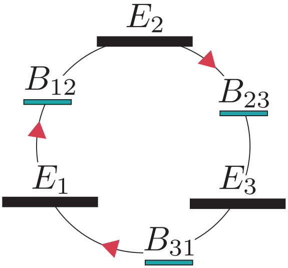
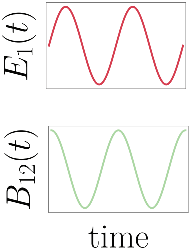
NEW YORK UNIVERSITY

Generating currents with periodic pumping

The "stochastic pumping" phenomenon.





Finite state Markov jump process
(or a diffusion process)

Detailed balanced
time-dependent rates
$W_{ij}(t) = e^{B_{ij}(t) - E_j(t)}$.

Pumping energy levels and barrier heights drives the system *out of equilibrium* $\implies$ non-zero average currents.

Stochastic pumps at the level of averages

To generate a current: *vary at least one energy level and one barrier*.

- No-pumping theorems: Sinitsyn [2009], Mandal and Jarzynski [2011].
- Geometric characterization of adiabatic pumping: Sinitsyn and Nemenman [2007], Rahav et al. [2008].

Less is known about **fluctuations and large deviations.**

Deviations away from the periodic steady state

Scaled cumulant generating function for σ, the total entropy production,

$$\psi_\sigma(\lambda) = \lim_{t\to\infty} t^{-1} \ln\langle e^{-\lambda\sigma}\rangle$$
$$= \lim_{t\to\infty} t^{-1} \ln \sum_{ij} \int_0^t W_{ij}(t;\lambda)\rho_j(t)$$

where $W_{ij}(t;\lambda)$ is the tilted generator for the entropy production at time t.

Deviations away from the periodic steady state

Settles into a time periodic steady state with period τ.

$$\begin{aligned}
\psi_\sigma(\lambda) &= \lim_{t\to\infty} t^{-1} \ln \sum_{ij} \int_0^t W_{ij}(t;\lambda)\rho_j(t) \\
&= \lim_{N\to\infty} (N\tau)^{-1} \sum_N \ln \sum_{ij} \int_0^\tau W_{ij}(t;\lambda)\rho_j(t) \\
&= \tau^{-1} \ln \int_0^\tau W_{ij}(t;\lambda)\rho_j^{\mathrm{ps}}(t)
\end{aligned}$$

Open question: What assumptions are necessary to prove the existence of an LDP for a periodically driven system?

Coarse-graining to a nonequilibrium steady state

Difficult to work with analytically, but we can try to coarse-grain.

Zia and Schmittmann [2007] $\Longrightarrow$ "Dynamical equivalence principle"

$$W^{\mathrm{ss}} = (\mathcal{S} + \mathcal{A})\mathcal{P}^{-1}$$

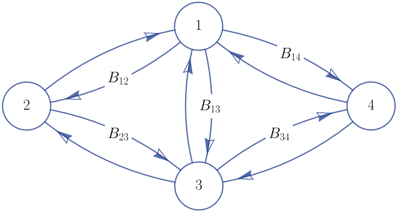
$$\mathcal{A}_{ij} = \frac{1}{2}\hat{j}_{ij}$$

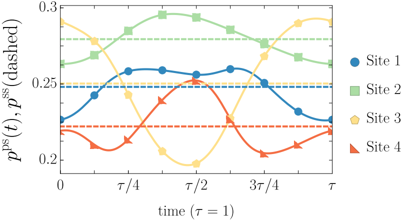
$$\mathcal{P}_{ii} = \hat{\rho}_i.$$

The symmetric part $\mathcal{S}$—unconstrained.

Choose it to match the average entropy production Raz et al. [2016]

Simple example: Four state network



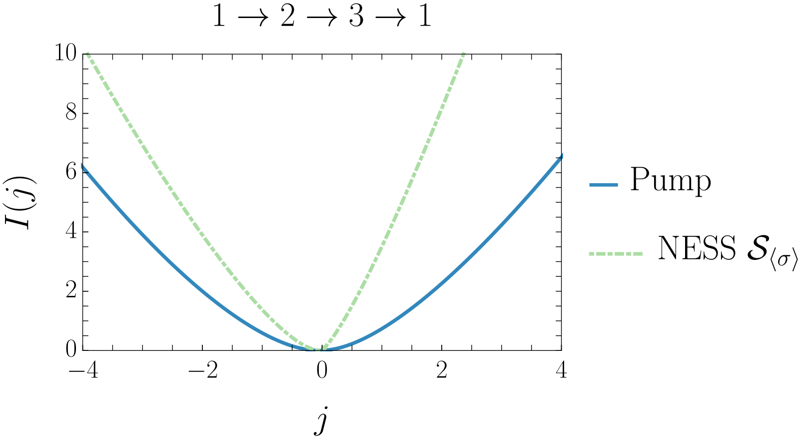


Periodic pumping protocol:

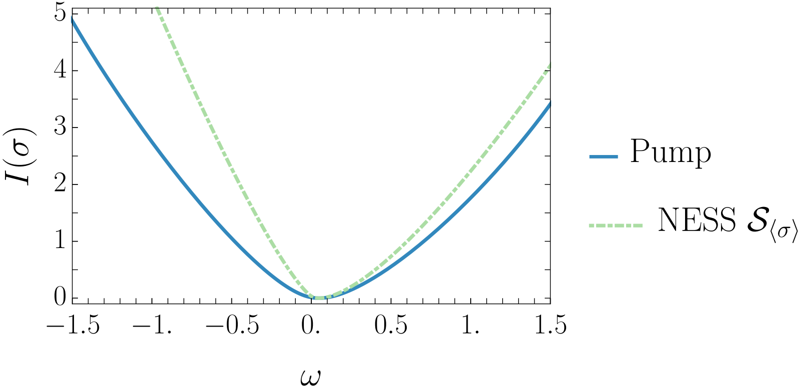
$$E_3(t) = \sin(2\pi t/\tau)$$

$$B_{13}(t) = 1 + \sin(2\pi t/\tau)$$

Fluctuations under coarse-graining?



Fluctuations under coarse-graining?



Level 2.5 Large Deviations

A different perspective on dynamical equivalence...
Empirical density:

$$\rho_i(t) = t^{-1} \int_0^t \delta(x(t') - x_i)\, dt'$$

Empirical flow:

$$q_{ji}(t) = t^{-1} \int_0^t \delta(x(t^-) - x_i)\delta(x(t^+) - x_j)\, dt'$$

For NESS with rate matrix W, an exact expression is known:

$$I(\boldsymbol{\rho}, \boldsymbol{q}) = \sum_{ij} W_{ij} p_j - q_{ij} + q_{ij} \ln \frac{q_{ij}}{W_{ij} p_j},$$

when $\boldsymbol{q}$ is conservative; cf. Maes and Netočny [2008].

Contract to get rate functions for currents

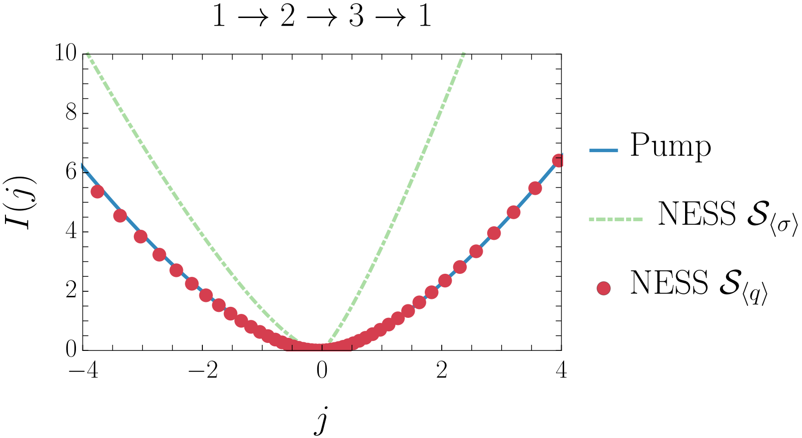
Contraction principle,

$$I(\boldsymbol{\rho}, \boldsymbol{j}) = \inf_{\boldsymbol{q},\ q_{ij}-q_{ji}=j_{ij}} I(\boldsymbol{\rho}, \boldsymbol{q}).$$

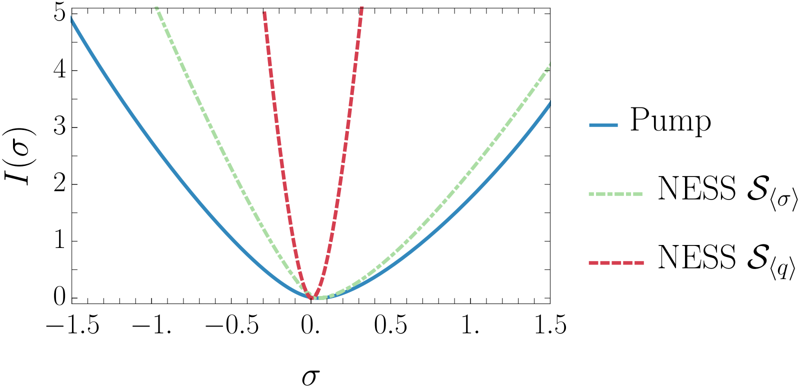
Ideas related to contraction play a role in proof of "Thermodynamic Uncertainty Relations" Gingrich et al. [2016].

- Does such a bound hold for periodic driving?
- What is the level 2.5 function for a periodically driven dynamics?

Fluctuations under coarse-graining?



Fluctuations under coarse-graining?



Degraded agreement for entropy production?

$$\sigma^{\text{pump}} = \tau^{-1} \int_0^\tau j_{ij}(t) \ln \frac{q_{ij}(t)}{q_{ji}(t)} dt$$

Split this into two, physical contributions,

$$\underbrace{\sigma^{\text{ss}}}_{\text{cycle part}} + \underbrace{\sigma^{\text{ex}}}_{\text{excess dissipated work}}$$

Similar to decompositions in the literature Esposito and Van den Broeck [2010]. Both entropy productions are positive on average.

Floquet decomposition approach

Fourier decomposition of the Master equation $\implies$

$$\partial_t p_i^{\mathrm{ps}}(t) = \hat{W}_{ij} p_j^{\mathrm{ps}}(t) + \mathcal{O}(k)$$

This is distinct from the period-to-period propagator,

$$\begin{aligned} p(t+\tau) &= \overline{\exp}\left(\int_t^{t+\tau} dt' W(t')\right) p(t) \\ &\equiv \mathcal{G}(\tau) p(t) \end{aligned}$$

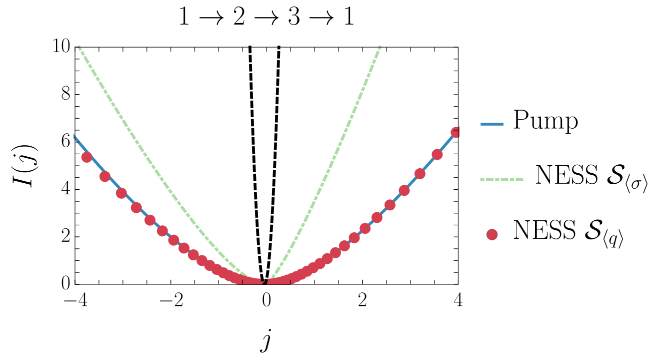
We cannot simply use the “stroboscopic” generator.

Consequence for uncertainty relations

In the weakly perturbed limit, for any current $\boldsymbol{j}$,

$$I^{\text{pump}}(\boldsymbol{j}) \leq \frac{(\boldsymbol{j} - \hat{\boldsymbol{j}})^2}{4\hat{\boldsymbol{j}}/\sigma^{\text{ss}}}.$$

Tighter quadratic bound than σ^{pump}.



Discrete time Markov Chains

A distinct bound exists for time-symmetric driving, cf. recent work of Proesmans and van den Broeck.

$$\frac{\hat{j}^2}{\hat{\delta j}^2} \leq \frac{1}{2\tau}\left(e^{\sigma} - 1\right)$$

Derivation relies on a large deviation function for flows based on Sanov's theorem:

$$\sum_{\Gamma} q_{\Gamma} \ln \frac{q_{\Gamma}}{p_{\Gamma}} - \sum_{k} q_k \ln \frac{q_k}{p_k}$$

Is this expression rigorously provable?

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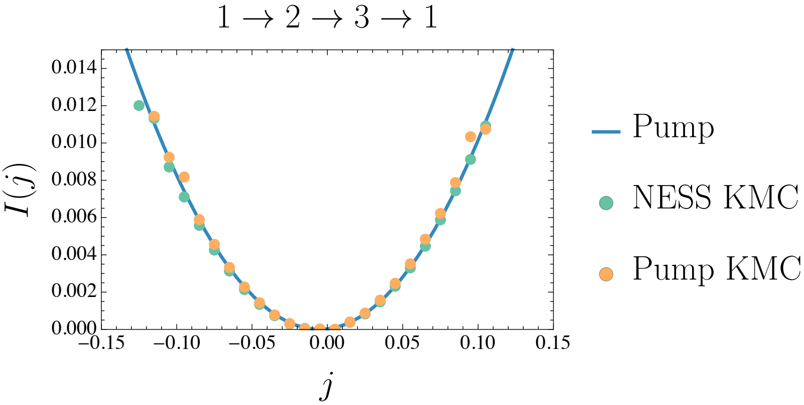
Kinetic Monte Carlo Sampling



References I

N A Sinitsyn. The stochastic pump effect and geometric phases in dissipative and stochastic systems. *J. Phys. A*, 42(19):193001, 2009. doi: 10.1088/1751-8113/42/19/193001.

Dibyendu Mandal and Christopher Jarzynski. A proof by graphical construction of the no-pumping theorem of stochastic pumps. *J. Stat. Mech. Theor. Exp.*, 2011(10):P10006, 2011. doi: 10.1088/1742-5468/2011/10/P10006.

N A Sinitsyn and I Nemenman. The Berry phase and the pump flux in stochastic chemical kinetics. *Euro. Phys. Lett.*, 77(5):58001, March 2007. doi: 10.1209/0295-5075/77/58001.

Saar Rahav, Jordan Horowitz, and Christopher Jarzynski. Directed Flow in Nonadiabatic Stochastic Pumps. *Phys. Rev. Lett.*, 101(14):140602, October 2008. doi: 10.1103/PhysRevLett.101.140602.

RKP Zia and B Schmittmann. Probability currents as principal characteristics in the statistical mechanics of non-equilibrium steady states. *J. Stat. Mech. Theor. Exp.*, 2007(07):P07012, 2007. doi: 10.1088/1742-5468/2007/07/P07012.

O Raz, Y Subaşı, and C Jarzynski. Mimicking Nonequilibrium Steady States with Time-Periodic Driving. *Phys. Rev. X*, 6(2):021022, May 2016. doi: 10.1103/PhysRevX.6.021022.

Christian Maes and Karel Netočný. Canonical structure of dynamical fluctuations in mesoscopic nonequilibrium steady states. *Euro. Phys. Lett.*, 82(3):30003, 2008. doi: 10.1209/0295-5075/82/30003.

Todd R Gingrich, Jordan M Horowitz, Nikolay Perunov, and Jeremy L England. Dissipation Bounds All Steady-State Current Fluctuations. *Phys. Rev. Lett.*, 116(12):120601, March 2016. doi: 10.1103/PhysRevLett.116.120601.

Massimiliano Esposito and Christian Van den Broeck. Three faces of the second law. I. Master equation formulation. *Phys. Rev. E*, 82(1):011143, 2010. doi: 10.1103/PhysRevE.82.011143.