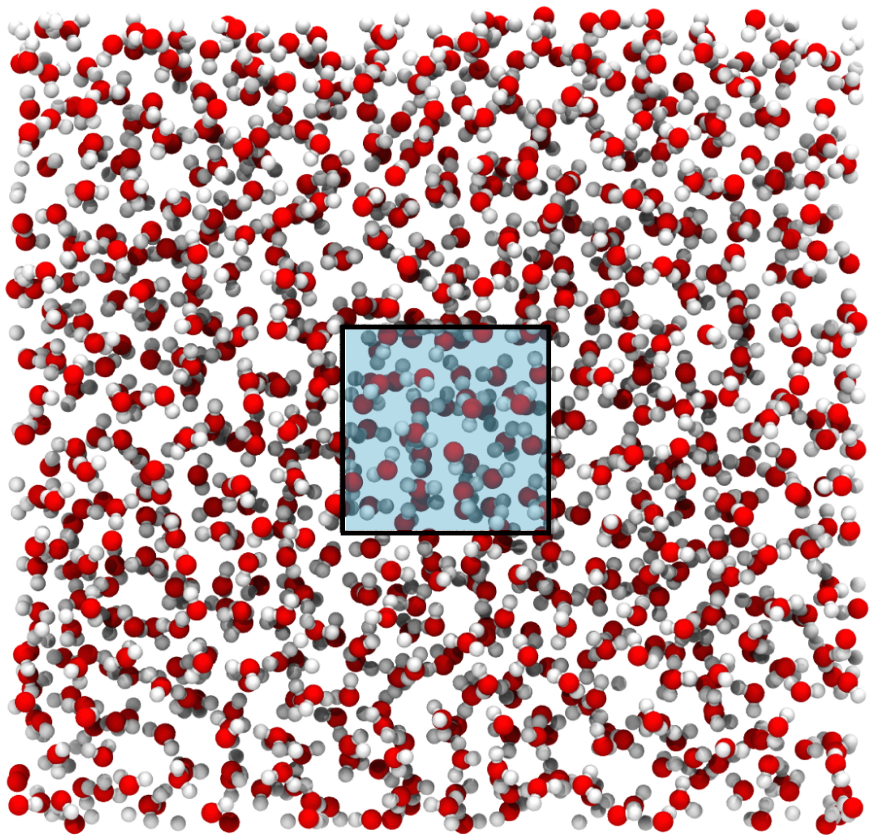
Levels without loops

A Pedagogical Overview of Large Deviation Theory in Nonequilibrium Statistical Physics

Grant Rotskoff
LINeq Meeting
Apr. 29th, 2016

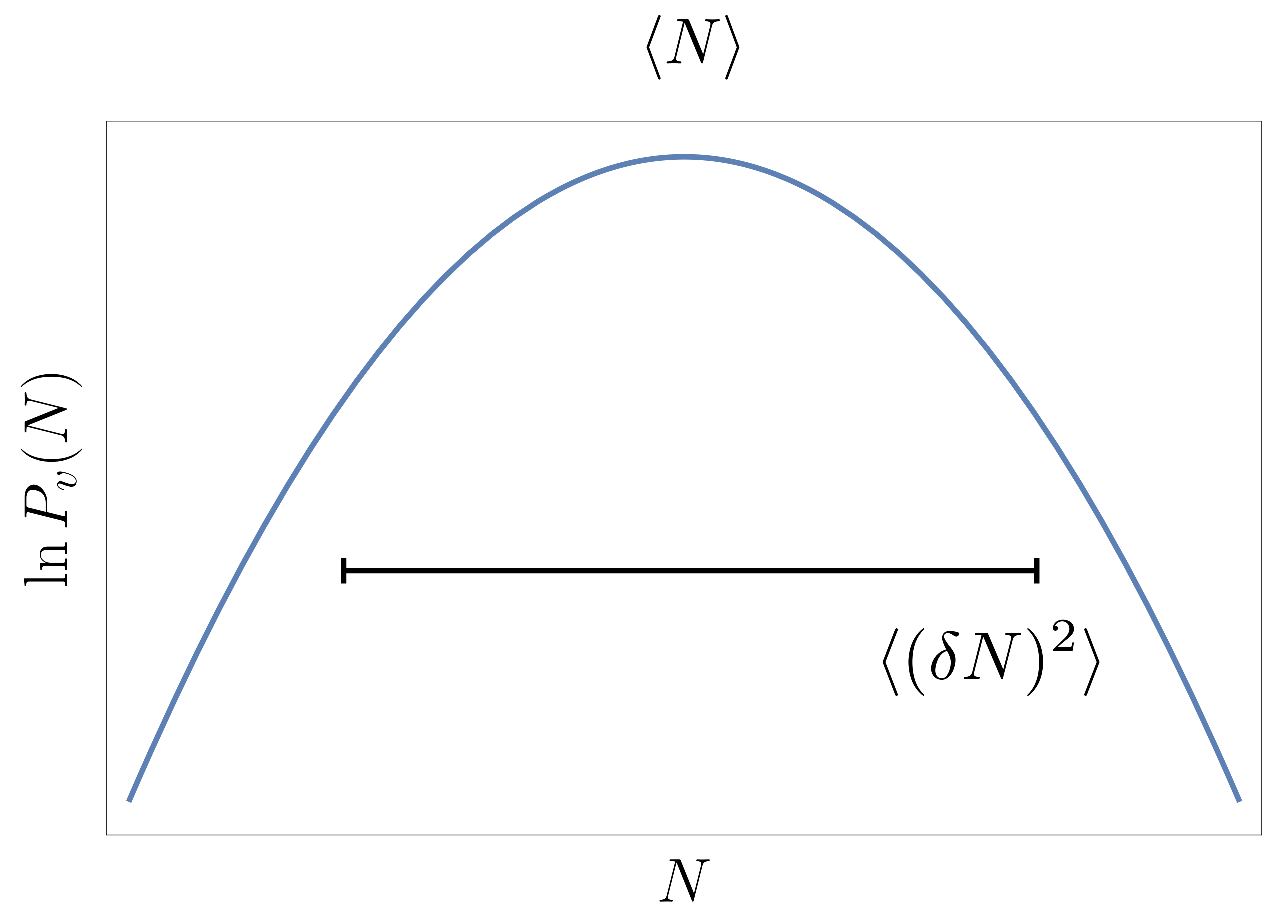
Small Deviations

Count the number of molecules



$N_v,$ number of molecules in the volume v

Typical fluctuations — Classical CLT



$$\text{Number of observations of } N_v \to \infty \implies -\ln P_v(N) \propto \frac{(N - \langle N \rangle)^2}{2\sigma^2}$$

$$\sigma^2 \sim (\text{Number of observations})^{-1}$$

Large Deviations

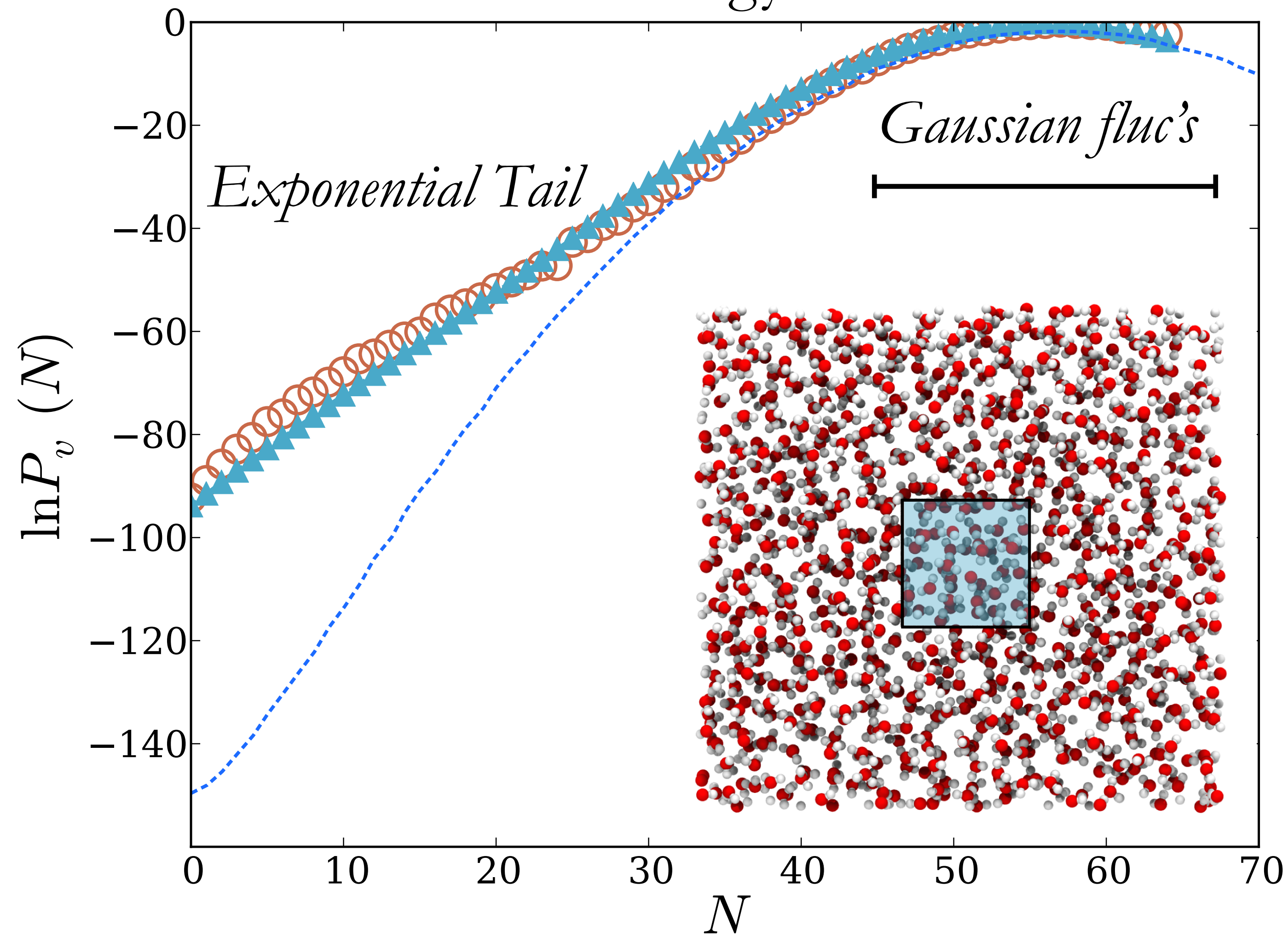
Physical properties are often determined by extreme rare events.

Central Limit Theorem does not describe this behavior.

Goal of Large Deviation Theory

What is the asymptotic form of the *full* probability distribution?

Solvation free energy as a rare event.



$$P(N_v) \asymp e^{n_{\text{obs}} I(N_v) + o(n_{\text{obs}})}$$

$\asymp$ denotes asymptotic equivalence

D. Chandler, Nature 437, 640 (2005).

S. Vaikuntanathan et al, Proc. Natl. Acad. Sci. U.S.A. 201513659 (2016).

Nonequilibrium observables in small systems

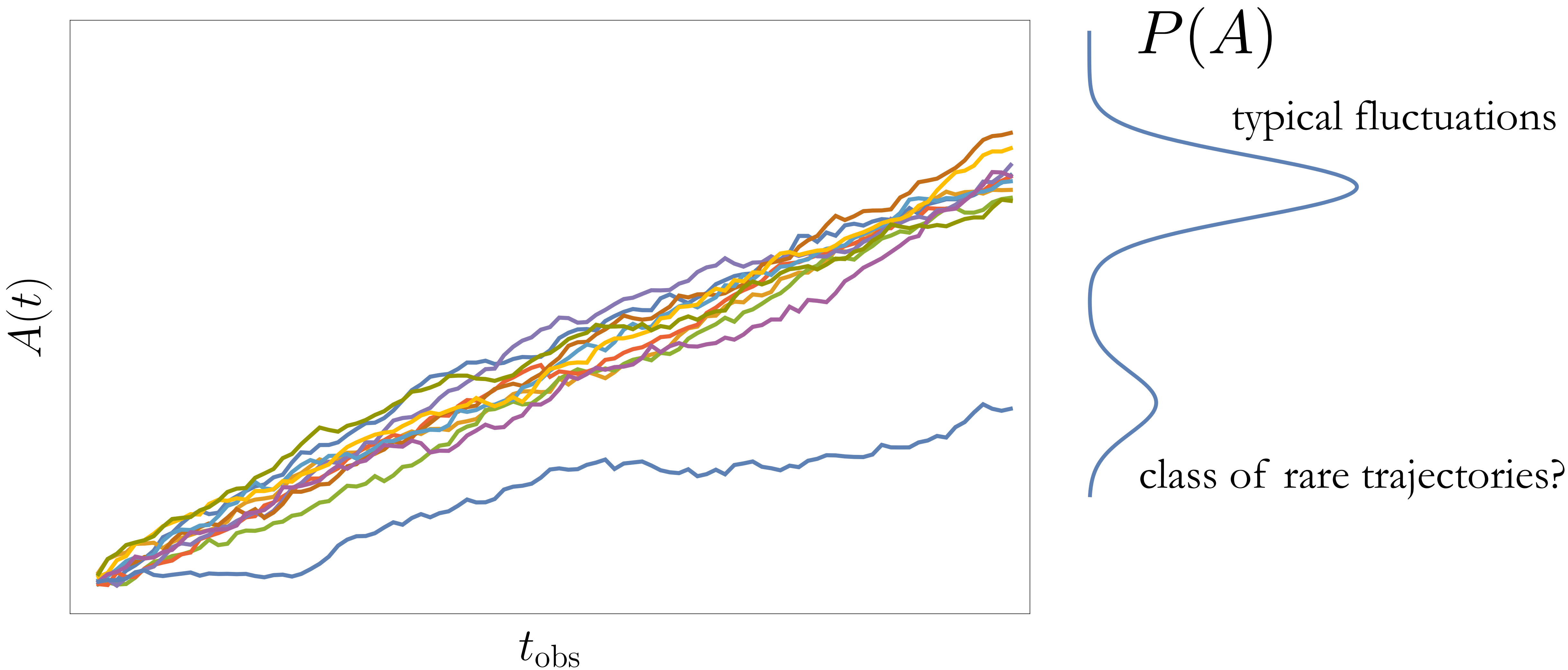
Thermodynamic Quantities

Work, Heat, Entropy Production

Dynamical Observables

Activity, Current

Common theme: time additivity
The trajectories, not configurations, are essential



Part I: Dynamical Free Energies

Key papers

[1] R. Chetrite and H. Touchette, Phys. Rev. Lett. 111, 120601 (2013).

[2] J. L. Lebowitz and H. Spohn, Journal of Statistical Physics (1999).

[3] J. P. Garrahan, et al, Phys. Rev. Lett. 98, 195702 (2007).

Reviews / Books

[1] H. Touchette, Physics Reports 478, 1 (2009).

[2] R. Ellis, Entropy, Large Deviations, and Statistical Mechanics.

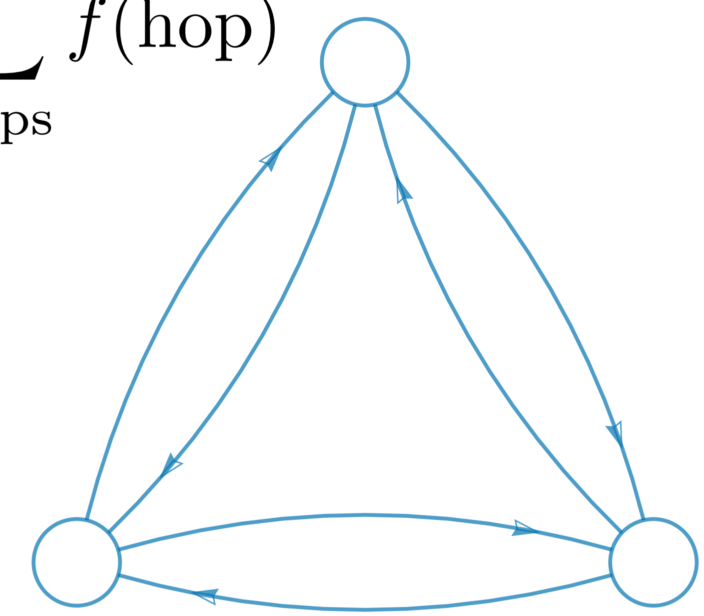
[3] M. I. Freidlin and A. D. Wentzell, Random Perturbations of Dynamical Systems.

The scaled cumulant generating function

$$\psi_\omega(k) = \lim_{t_{\text{obs}}\to\infty} \frac{1}{t_{\text{obs}}} \ln \left\langle e^{k\omega(t)} \right\rangle$$

dynamical observable

$$\omega(t_{\text{obs}}) = \sum_{\text{hops}} f(\text{hop})$$



Example: Ergodic Markov Process

Perron Frobenius $\Longrightarrow$ unique stationary distribution

$$\left\langle e^{k\omega} \right\rangle = \sum_{\text{States, } x_i} p_{\text{ss}}(x_1) e^{k\omega^{x_1 \to x_2}} \pi(x_2|x_1) \times \cdots \times e^{k\omega^{x_{n-1}\to x_n}} \pi(x_n|x_{n-1})$$

"Tilted" transition matrix with: $\pi_k^{\text{tilted}}(x_2|x_1) = e^{k\omega^{x_1\to x_2}} \pi(x_2|x_1)$

Long time limit determined by the maximum eigenvalue,

$$\psi_\omega(k) = \ln \max \operatorname{eig} \mathbb{T}_k^{\text{tilted}}$$

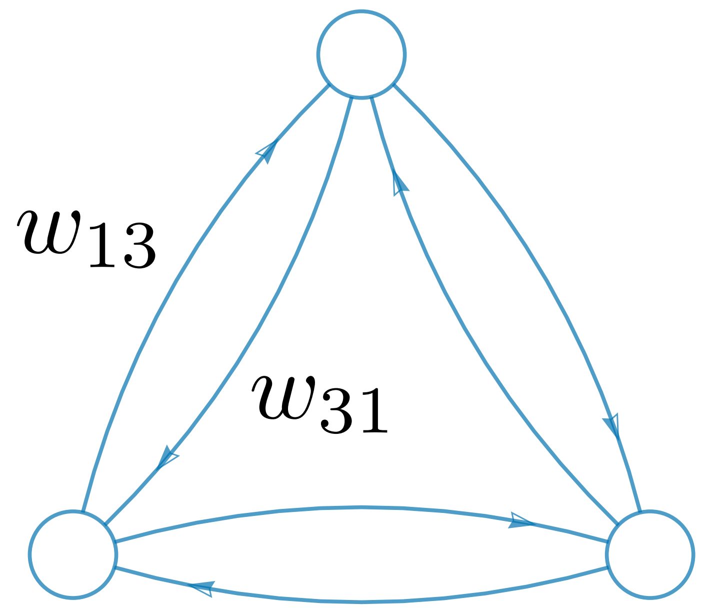
Entropy production tilted operator

For a single transition,

$$\omega(i \to j) = \ln \frac{w_{ji}}{w_{ij}}$$

w_{ji} ⟵ Forward Rate

w_{ij} ⟵ Reverse Rate



$$\pi_k^{\text{tilted}}(x_j|x_i) = \underbrace{e^{k \ln w_{ji}/w_{ij}}}_{\text{entropy production tilt}} \pi(x_j|x_i) = w_{ji}^k w_{ij}^{1-k} \pi(x_j|x_i)$$

Application of the tilted generator:

Time reversal corresponds to transposition, and we can read off an entropy production fluctuation theorem

$$\psi_\omega(k) = \psi_\omega(1-k)$$

J. L. Lebowitz and H. Spohn, Journal of Statistical Physics (1999).

Generating functions as dynamical free energies

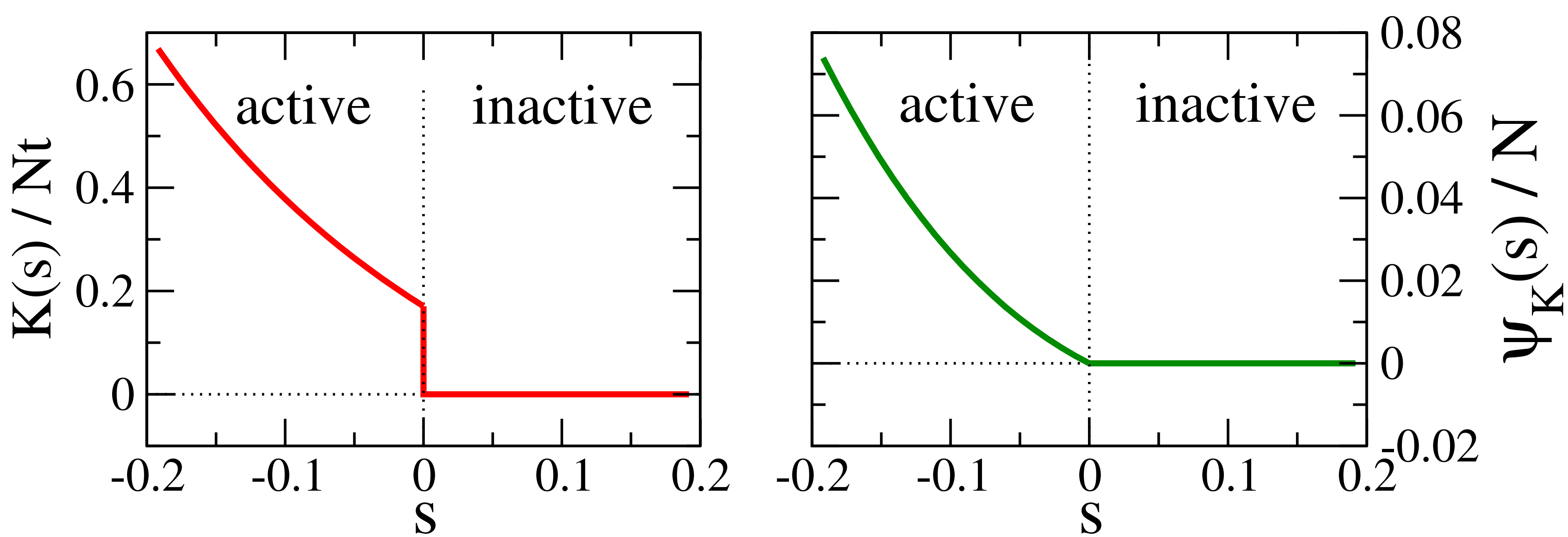
Equilibrium: free energies are SCGFs

$$f_{\text{canonical}} = -\frac{k_\text{B}T}{N} \ln \int d^d x \; e^{-\beta E(x)}$$
$$= -\frac{k_\text{B}T}{N} \ln \left\langle e^{-\beta N \epsilon(x)} \right\rangle$$

Nonequilibrium: the extensive quantities grow with time, not system size

$$f_{\text{noneq}} = \frac{1}{N} \ln \int_0^T \mathcal{D}[x(t)] P_{\text{traj}}[x(t)] e^{-kA(t)}$$

Example: Fluctuations in activity in models of glassy dynamics



J. P. Garrahan, et al, Phys. Rev. Lett. 98, 195702 (2007).

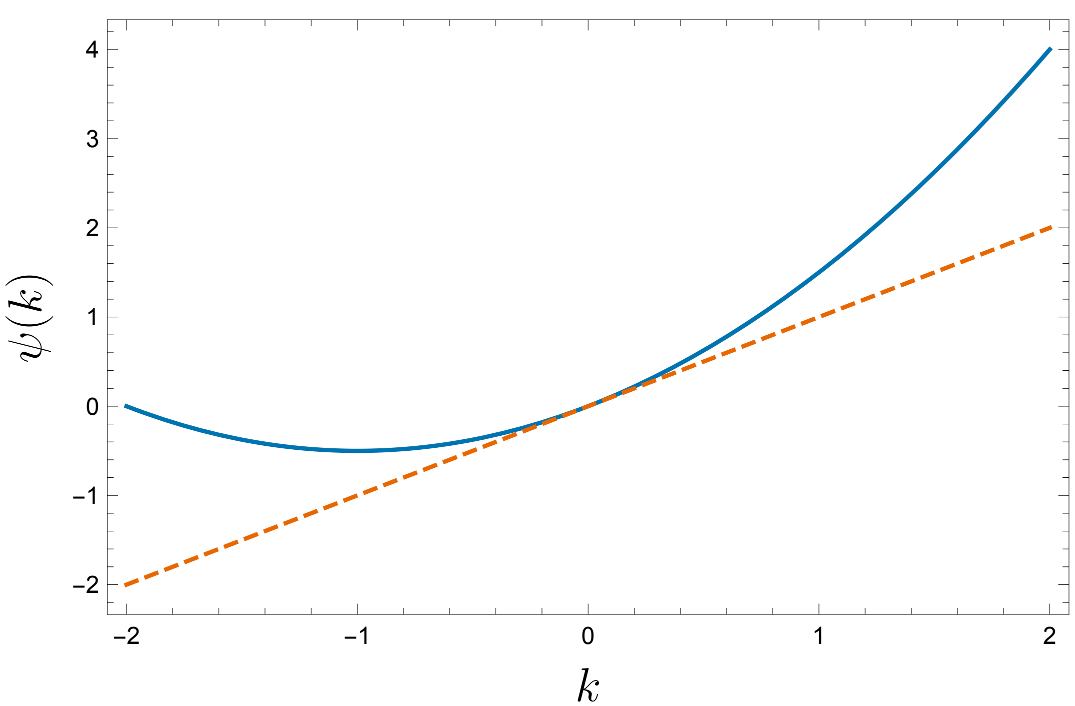
Rate Functions via Legendre Fenchel Transform

Gärtner-Ellis Theorem

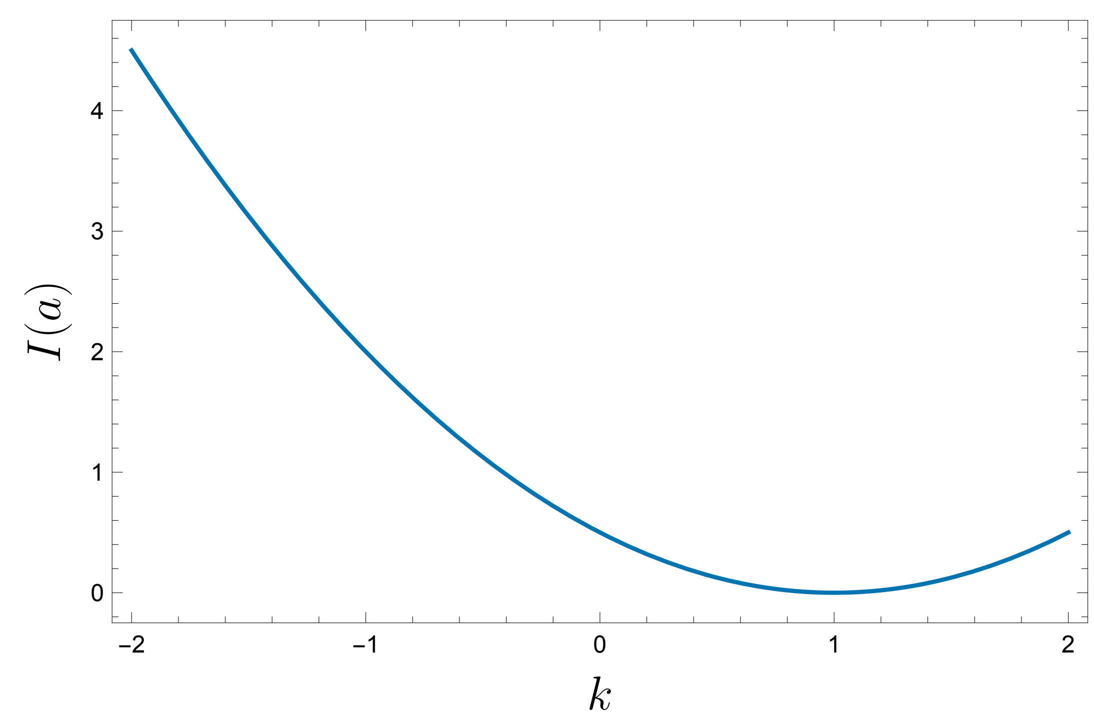
If the scaled cumulant generating function $\psi_A(k)$ exists and is differentiable for all k. Then A satisfies a large deviation principle, i.e.,

$$p(A/t_{\text{obs}} = a) \asymp e^{t_{\text{obs}} I(a)}$$

Slope at zero of the SCGF gives the average



"Rate Function" $I(a) = \sup_k [ka - \psi(k)]$

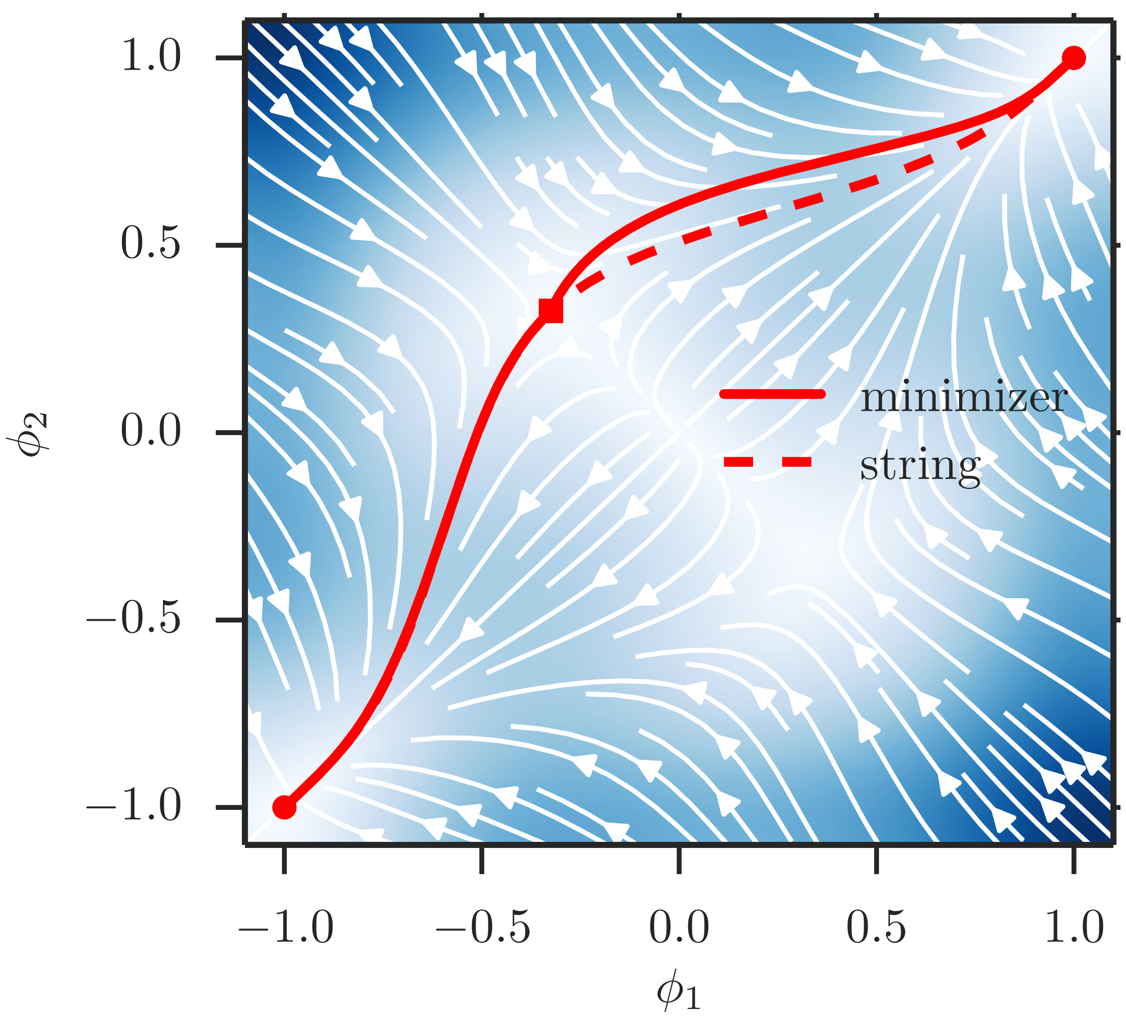


Low Noise Limit

"Friedlin-Wentzell Large Deviations"

$$dX_t = F(X_t)\ dt + \sqrt{\epsilon}\ dW_t$$
$$P[x(t)] \asymp \exp\left[\epsilon^{-1} I[x(t)]\right]$$

Solutions to the stochastic differential equations fluctuate around a minimum action path



Example: Overdamped, driven Brownian motion

$$\dot{x} = -\nabla V(x) + F + \eta$$

$$I[x(t)] = \int_0^{t_{\mathrm{obs}}} d\tau \ \left[\frac{1}{4}(\dot{x} + \nabla V - F)^2 - \frac{1}{2}\nabla^2 V\right]$$

T. Speck, A. Engel, and U. Seifert, J. Stat. Mech. 2012, P12001 (2012).

T. Grafke, T. Schaefer, and E. Vanden-Eijnden, arXiv math.NA, (2016).

Determining other rate functions

We want a rate function of some other observable

Contraction Principle $B = f(A)$

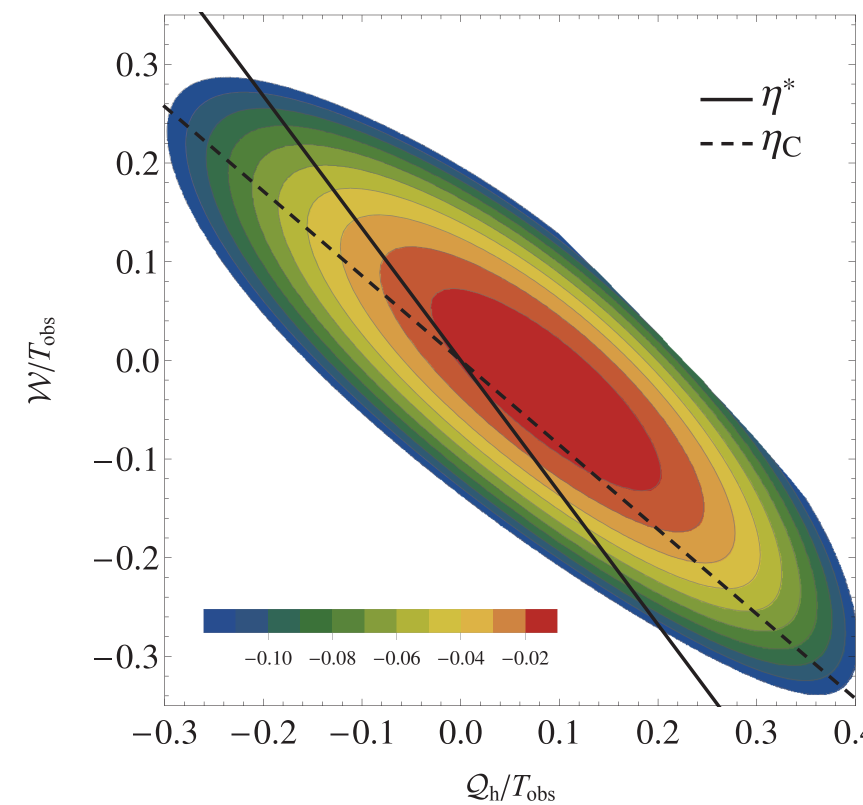
Suppose we know the rate function: $I_A(a)$

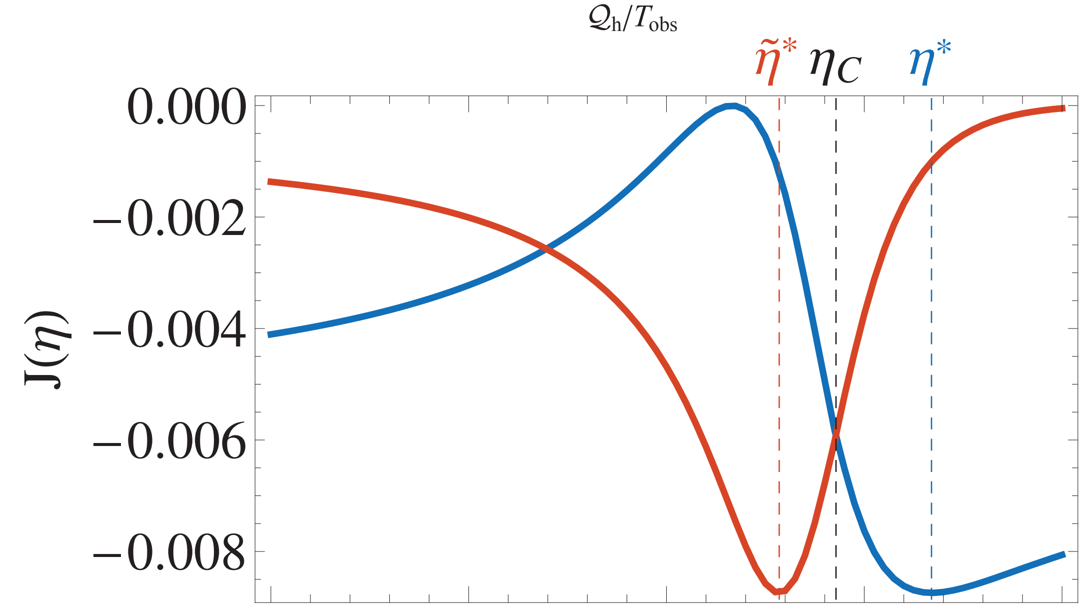
$$I_B(b) = \sup_{a:f(a)=b} I_A(a)$$

Analogous to a saddle point approximation

If an observable A satisfies a large deviation principle with rate function $I_A(a)$ then the image of A under a continuous map f also satisfies a large deviation principle.

Example: Efficiency rate function





Part II: The Level Abstraction

[1] A. C. Barato and R. Chetrite, Journal of Statistical Physics 160, 1154 (2015).

[2] C. Maes and K. Netočný, Euro. Phys. Lett 82, 30003 (2008).

[3] V. Y. Chernyak, et al, Journal of Statistical Physics 137, 109 (2009).

[4] L. Bertini et al, Annales De l'Institut Henri Poincaré, Probabilités Et Statistiques 51, 867 (2015).

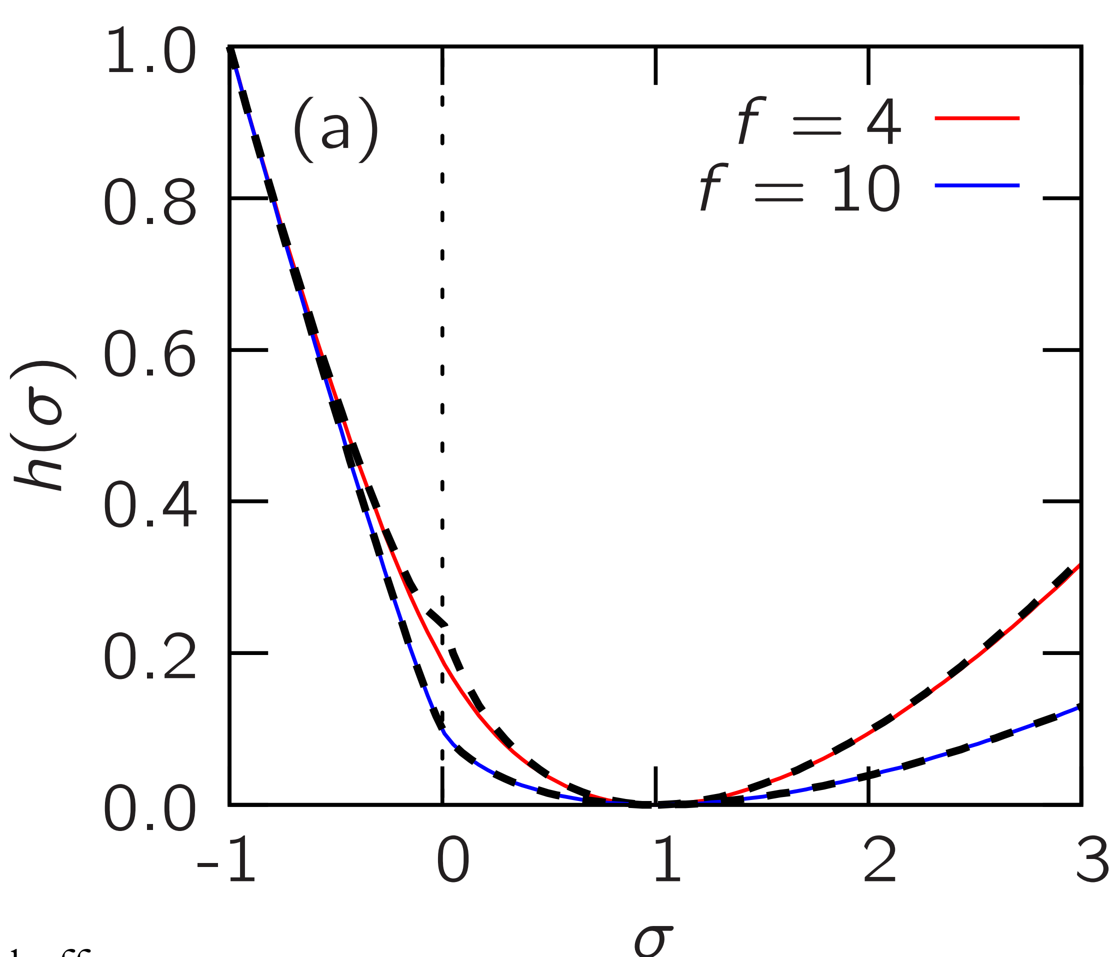
Level I—Rate functions for a given observable

extensive observable: $A[x(t)]$

$$P(A) \asymp e^{t_{\mathrm{obs}} I^{(1)}(A/t_{\mathrm{obs}})}$$

$$I^{(1)}(\langle A \rangle) = 0$$

The level I rate function
for an extensive observable A is
exactly the type of rate function we've
encountered thus far.



Example: Asymmetric Random Walk entropy production rate function

B. Derrida and J. L. Lebowitz, Phys. Rev. Lett. 80, 209 (1998).

Level II—Empirical Density

Fluctuations in the time spent in each state

$$\rho_{t_{\text{obs}}}(x) = \int_0^{t_{\text{obs}}} \delta(x(t) - x)\; dt$$

Can be used to compute level one rate functions for state-dependent observables

Higher level: can get any level I rate function by contraction

$$I_A^{(1)}(a) = \sup_{a: f(\rho)=a} I^{(2)}(\rho)$$

Example: Sanov's Theorem

Draw a random state vector. Then the rate function for the empirical measure is just the KL divergence.

$$\begin{aligned} I_\rho^{(2)}(\nu) &= \int \nu(dx) \frac{d\rho}{d\nu}(x) \\ &= D_{\text{KL}}(\rho \| \nu) \end{aligned}$$

Problem: Most of the observables we are interested depend on the dynamics.

Level II.5—Empirical Density + Currents

Monitor transitions in the system

$$C_{t_{\text{tobs}}}(x_i, x_j, \delta t) = \int_0^{t_{\text{obs}}} \delta(x(t) - x_i)\delta(x(t+\delta t) - x_j)\ dt$$

Remarkably, there is an explicit form for Markov jump processes at steady state

$$I^{(2.5)}[\rho, C] = \sum_{x,y} \rho(x)W(x,y) - C(x,y) + C(x,y) \ln \frac{C(x,y)}{\rho(x)W(x,y)}$$

And for diffusions (divergence free steady state currents)

$$I^{(2.5)}[\rho, j] = \int dx\ \frac{(j - j_{\text{ss}})^2}{\rho D}$$

Caveat: performing the contraction can be hard

C. Maes and K. Netočný, Euro. Phys. Lett 82, 30003 (2008).

A. C. Barato and R. Chetrite, Journal of Statistical Physics 160, 1154 (2015).

Thermodynamic Uncertainty Relations

Current fluctuations are bounded
by Gaussian entropy production fluctuations

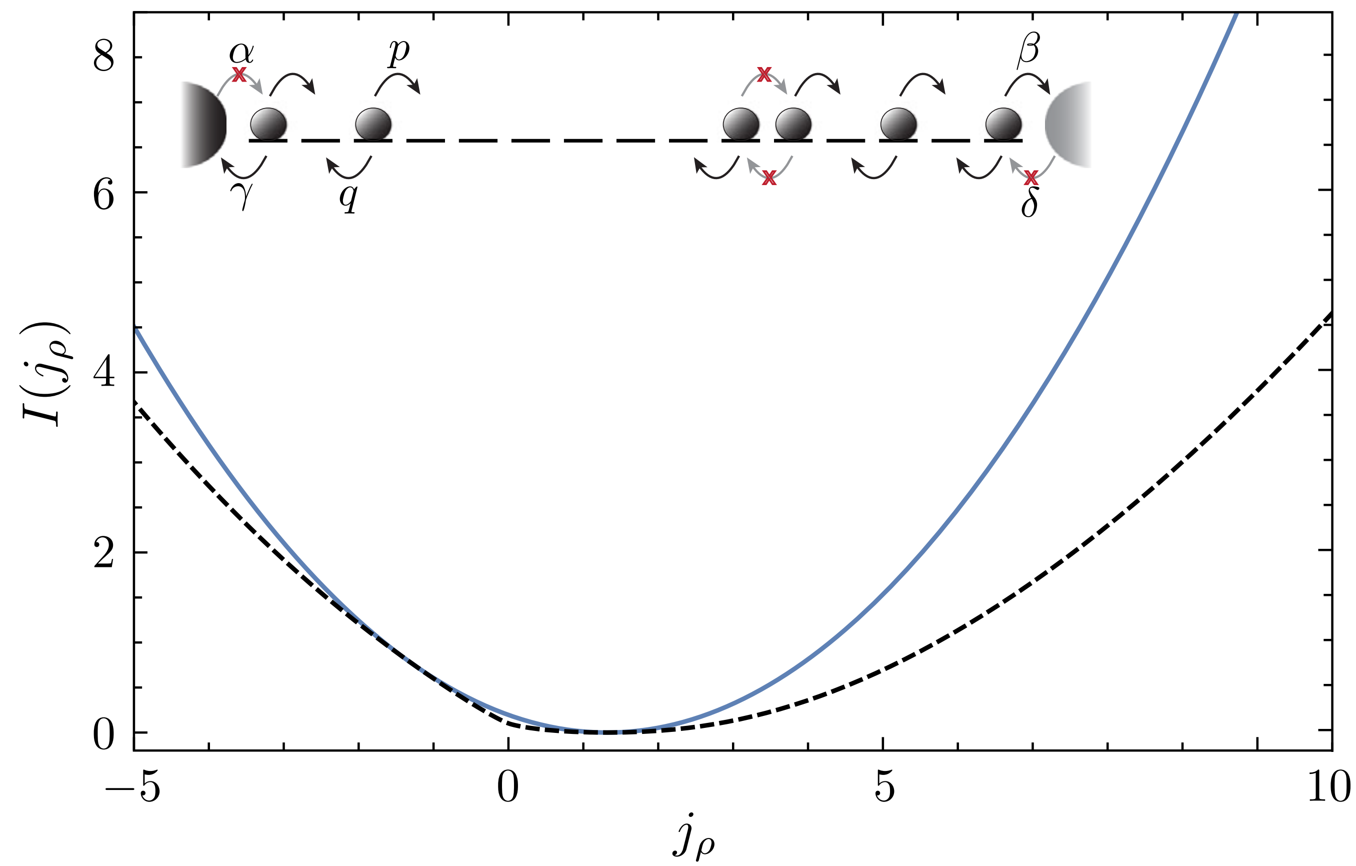
$$I(j) \leq I_{\mathrm{G}}(\omega)$$

Fluctuation Theorem symmetry for
Gaussian entropy production distribution

$$\mathrm{Var}(\omega) = 2\langle\omega\rangle$$

Direct consequence of the
Level II.5 rate function
for Markov jump processes

C.f., T. R. Gingrich, et al, Phys. Rev. Lett. 116, 120601 (2016).



A. C. Barato and U. Seifert, Phys. Rev. Lett. 114, 158101 (2015).

P. Pietzonka, A. C. Barato, and U. Seifert, arXiv (2015).

Extended Bibliography — Physics

In addition to the references throughout the talk, the following papers detail some applications of large deviation theory to the study of nonequilibrium systems. This list is woefully incomplete and draws heavily from a small corner of the full community working on these types of problems.

B. Derrida, J. Stat. Mech. 2011, P01030 (2011).

R. Chetrite and H. Touchette, Phys. Rev. Lett. 111, 120601 (2013).

P. I. Hurtado and P. L. Garrido, J. Stat. Mech. 2009, P02032 (2009).

R. L. Jack and P. Sollich, arXiv cond-mat.stat-mech, 2351 (2015).

V. Lecomte, et al, Journal of Statistical Physics 127, 51 (2007).

J. P. Garrahan, et al, J. Phys. a: Math. Theor. 42, 075007 (2009).

D. S. Dean and S. N. Majumdar, Phys. Rev. Lett. 97, 160201 (2006).

Extended Bibliography — Numerical Work

You can't do large deviation theory without a rate function. One of the most significant challenges in applying large deviation theory lies in the challenge of robustly computing the rate function from numerical simulations. This problem is especially important in cases where the generator is sufficiently complicate to preclude the use of spectral methods.

J. Tailleur, et al, in MODELING and SIMULATION of NEW MATERIALS: Proceedings of Modeling and Simulation of New Materials: Tenth Granada Lectures (AIP, 2008), pp. 212–219.

C. Giardina, J. Kurchan, and L. Peliti, Phys. Rev. Lett. 96, 120603 (2006).

T. Nemoto, F. Bouchet, R. L. Jack, and V. Lecomte, arXiv cond-mat.stat-mech, (2016).

V. Lecomte and J. Tailleur, J. Stat. Mech. 2007, P03004 (2007).

C. Giardina, J. Kurchan, V. Lecomte, and J. Tailleur, Journal of Statistical Physics 145, 787 (2011).