Geodesic optimization in thermodynamic control

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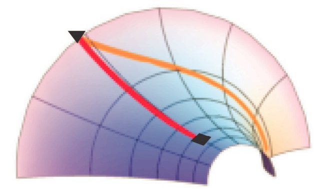
Some long-term goals:

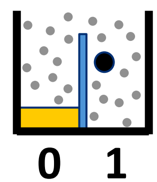
- New thermodynamic relations
- Predict signatures of efficient biomolecules
- Design optimal computational devices

Talk Outline

- Geometric framework



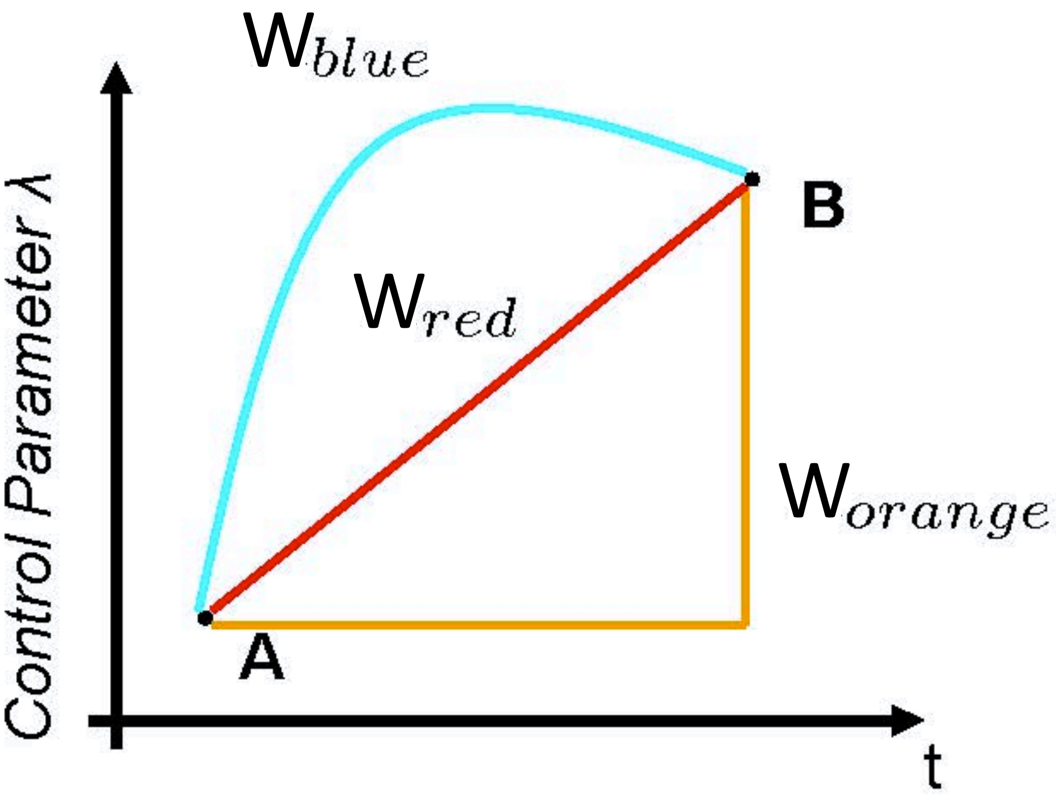
- Optimal bit erasure



- New generalization of geometric framework from Slow Perturbation Theory

Cost of a Protocol

Different protocols cost different amounts of work



Geometry in thermodynamics

- Long history, e.g.:

  Weinhold, J Chem Phys 63, 2479 (1975)
  Ruppeiner, PRA 20, 1608 (1979)
  Schlögl, Z Phys B 59, 449 (1985)
  Salamon, Nulton, & Ihrig, J Chem Phys 80, 436 (1984)
  Salamon & Berry, PRL 51, 1127 (1983)
  Brody & Rivier, PRE 51, 1006 (1995)

  ⋮

- "Thermodynamic length"
- Assumed endoreversibility (system in equilibrium, if not same as environment)
- Macroscopic description

Geometry in thermodynamics

- Microscopic rather than macroscopic:

  Crooks, PRL 99, 100602 (2007)
  Burbea & Rao, J. Multivariate Anal. 12, 575 (1982)
  Feng & Crooks, PRE 79, 012104 (2009)

- Extend to nonequilibrium systems (beyond endoreversibility):

  Sivak & Crooks, PRL 108, 190602 (2012)

- Derived in the linear response regime
- Since extended (Mandal & Jarzynski, others)

Linear resp. $\Rightarrow$ optimal protocols = geodesics

$$\langle \Delta \mathbf{X}(t_0) \rangle_\Lambda \simeq \int_{-\infty}^{t_0} dt' \underbrace{\boldsymbol{\chi}(t_0 - t') \cdot [\boldsymbol{\lambda}(t') - \boldsymbol{\lambda}(t_0)]}$$

Conjugate forces

$$\mathbf{X} \equiv -\partial E / \partial \boldsymbol{\lambda}$$

$$\Delta \mathbf{X}(t_0) \equiv \mathbf{X}(t_0) - \langle \mathbf{X} \rangle_{\boldsymbol{\lambda}(t_0)}$$

$$\chi_{ij}(t) \equiv \beta \frac{d}{dt} \langle \delta X_j(0) \delta X_i(t) \rangle_{\boldsymbol{\lambda}(t_0)}$$

$$\Downarrow$$

External control parameters

Riemannian Metric

$$\mathcal{P}_{\mathrm{ex}}(t_0) = \left[\frac{d\boldsymbol{\lambda}^T}{dt}\right]_{t_0} \cdot \zeta(\boldsymbol{\lambda}(t_0)) \cdot \left[\frac{d\boldsymbol{\lambda}}{dt}\right]_{t_0}$$

$$\zeta_{ij}(\boldsymbol{\lambda}(t_0)) = \beta \int_0^\infty dt'' \langle \delta X_j(0) \delta X_i(t'') \rangle_{\boldsymbol{\lambda}(t_0)}$$

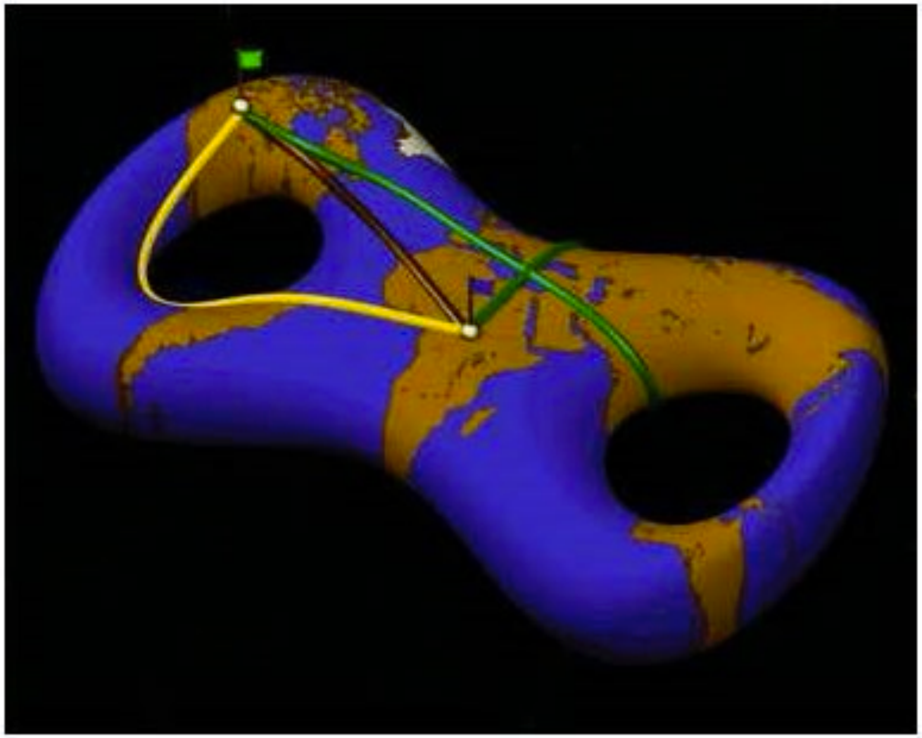
Sivak & Crooks, PRL (2012)

Some properties of optimal protocols (in linear resp. regime):

- Follow geodesics
- Require constant excess power
- Independent of total duration except for global rescaling
- Can be calculated based on equilibrium aspects of system

Sivak & Crooks, PRL (2012)

Optimal protocols are geodesics



(Even simple geometries can yield complex optimal protocols in terms of the control parameters)

Once you know the metric, how do you find geodesics?

No systematic way that's guaranteed to work, but there are tools:

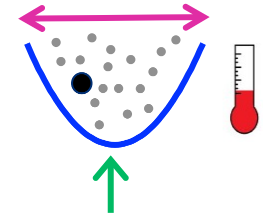
- Christoffel symbols
- Geodesic equation
- Scaler curvature (Ricci scaler; useful in 2-D)
- Killing vector fields (isometries/symmetries)
- Try various coordinate transformations to simplify eqs., and recognize familiar spaces

1^{st} model: Particle in optical tweezers

(or driven torsion pendulum, or nanomechanical oscil.)

Inertial Langevin dynamics, 3 control params:

Zulkowski, Sivak, Crooks & DeWeese PRE (2012)

1st model: Particle in optical tweezers 

Inertial Langevin dynamics:

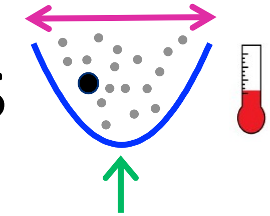
$$m\,\ddot{y} + k(t)[y - y_0(t)] + \zeta^c\,\dot{y} = F(t)$$

with Gaussian white noise:

$$\langle F(t)\rangle = 0\,,\ \langle F(t)F(t')\rangle = \frac{2\zeta^c}{\beta(t)}\delta(t - t')$$

Zulkowski, Sivak, Crooks & DeWeese PRE (2012)

1st model: Particle in optical tweezers



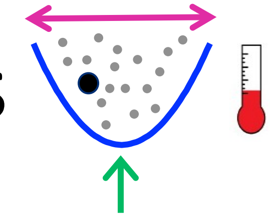
- Decoupling of y_0 from (β, k)

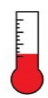
Metric tensor:

$$
\begin{array}{cccc}
 & y_0 & \beta & k \\
g_{ij} = \dfrac{m}{4\zeta^c} & \left(\begin{array}{ccc}
\frac{4(\zeta^c)^2}{m}\beta & 0 & 0 \\
0 & \frac{1}{\beta^2}\left(4 + \frac{(\zeta^c)^2}{km}\right) & \frac{1}{\beta k}\left(2 + \frac{(\zeta^c)^2}{km}\right) \\
0 & \frac{1}{\beta k}\left(2 + \frac{(\zeta^c)^2}{km}\right) & \frac{1}{k^2}\left(1 + \frac{(\zeta^c)^2}{km}\right)
\end{array}\right) & \begin{array}{c} y_0 \\ \beta \\ k \end{array} &
\end{array}
$$

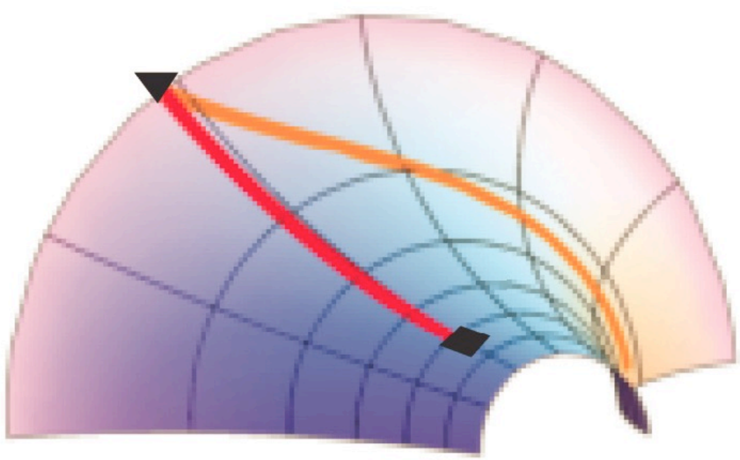
Zulkowski, Sivak, Crooks & DeWeese PRE (2012)

1st model: Particle in optical tweezers



1/ 

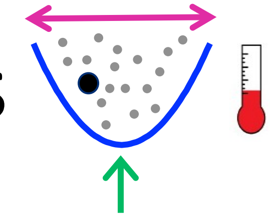
(d)



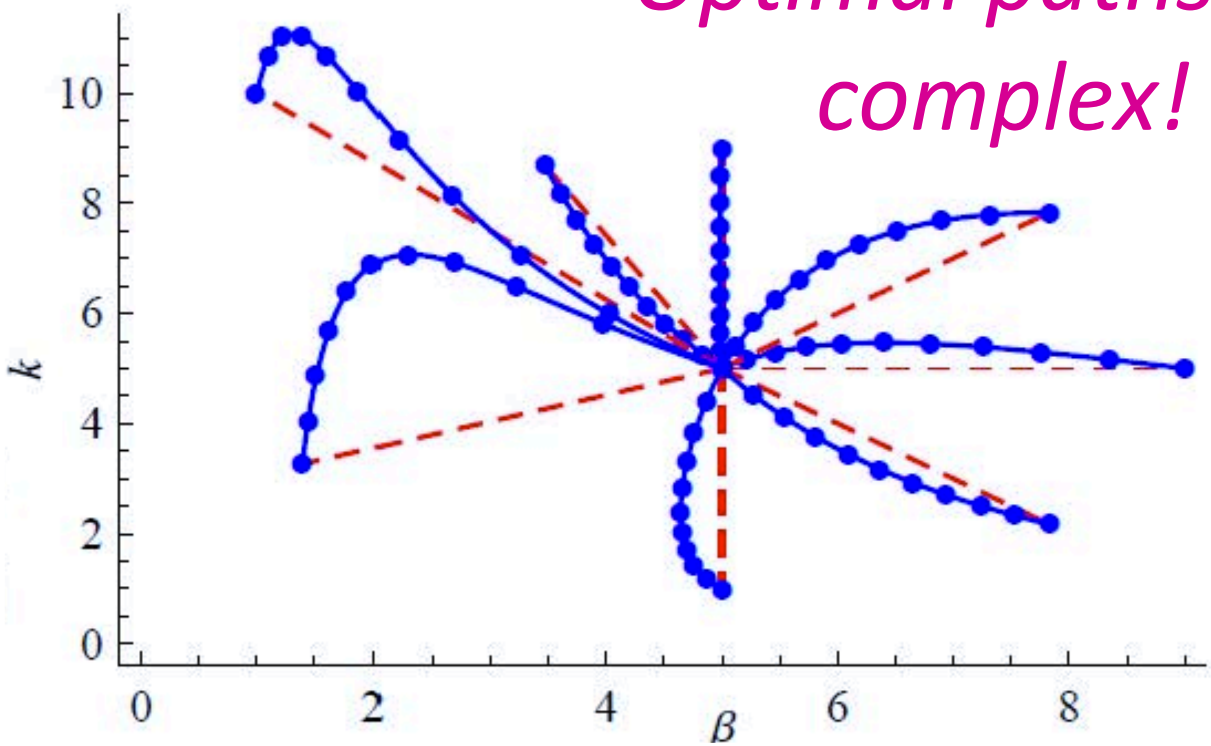
Change of variables:
hyperbolic geometry

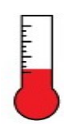
Zulkowski, Sivak, Crooks & DeWeese PRE (2012)

1st model: Particle in optical tweezers



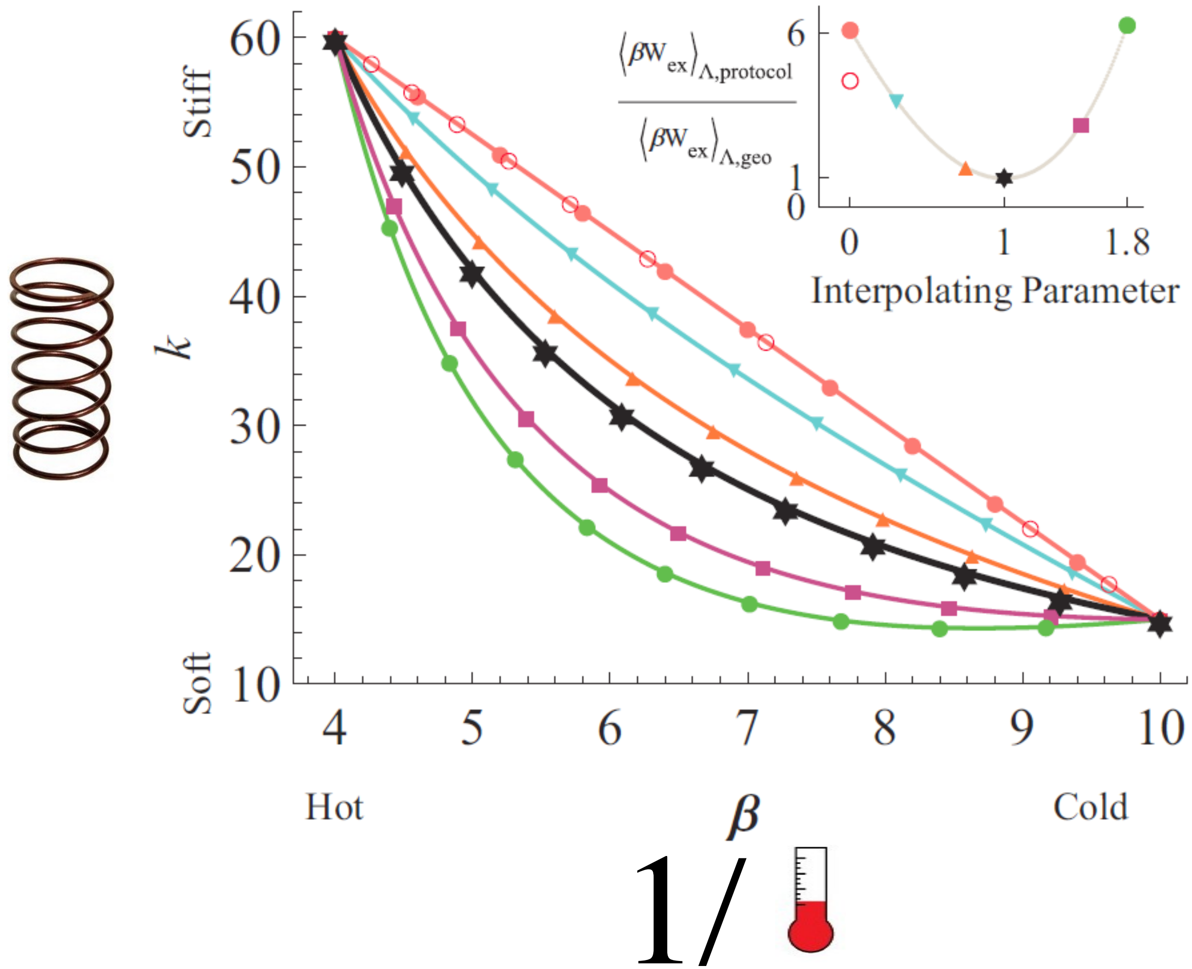
Optimal paths are complex!



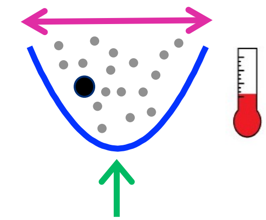
1/ 

Zulkowski, Sivak, Crooks & DeWeese PRE (2012)

Optimal protocol can be much more *efficient* than nearby paths



Notes and open questions:



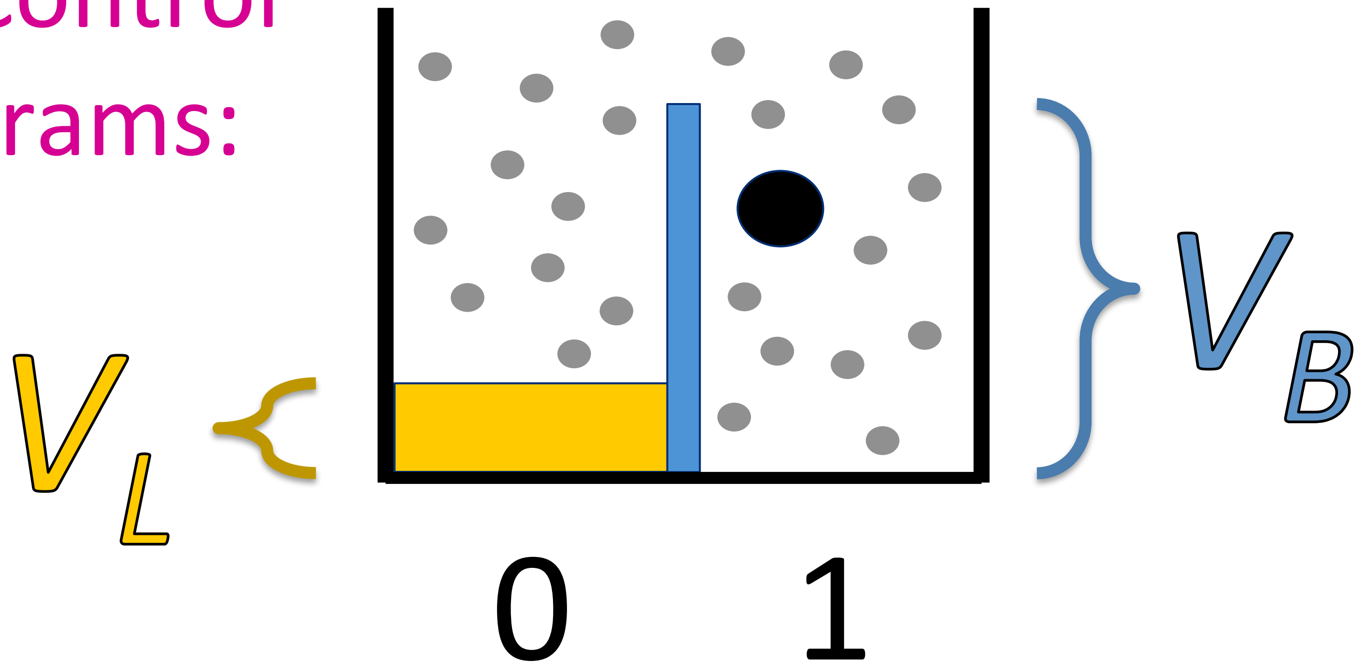
- Can optimize 3 params at once
  (k, y_0: Aurell 2012; Seifert 2007, 2008)
- Treating β as a control parameter; measuring dissipation in units of entropy
- What do the 2 conserved quantities mean?
- Are there more? (can be up to 6 Killing fields)
- What is full range of applicability for this approach? (> lin. resp. & deriv. truncation?)
- What does scalar curvature (R) represent?
  (seems different than R of George Ruppeiner, but
  P.S. Krishnaprasad calc. suggests deep connection…)

Optimal bit erasure:
a simple, but exactly solvable, model

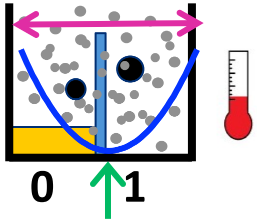
a simple, but exactly solvable, model

Overdamped, Brownian particle in double square well; Fokker-Planck for geometric approach

2 control params:



Optimal bit erasure



Flat manifold!

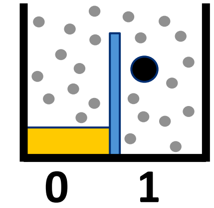
vanishes everywhere
for this 2-D model:

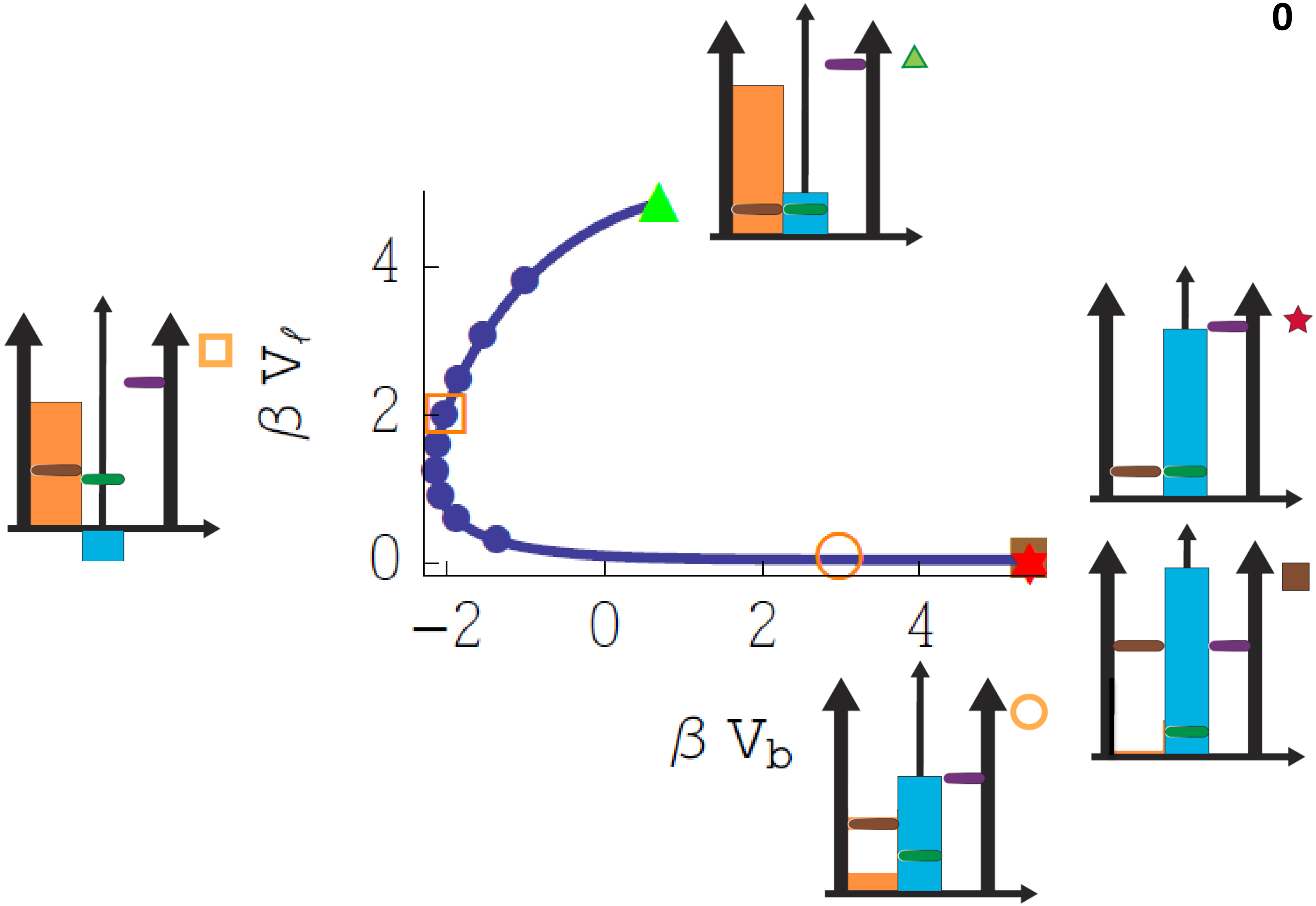
$$R = 0$$

Flat manifold!

Zulkowski & DeWeese PRE (2014)

Optimal bit erasure





Zulkowski & DeWeese PRE (2014)

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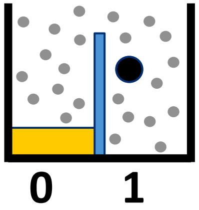
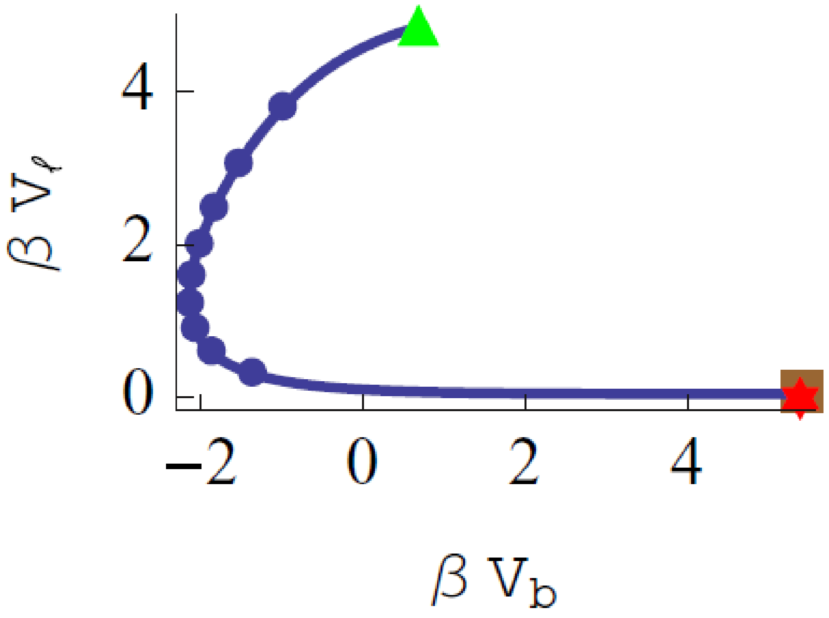
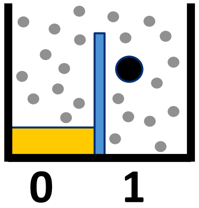


Exact:



Zulkowski & DeWeese PRE (2014)

Optimal bit erasure



$$\langle \beta Q \rangle_{\Lambda_{\mathrm{opt}}} \approx \frac{-\Delta S}{k_B} + \frac{4K}{\bar{t}_f}$$

Landauer *Finite t cost*

Aurell et al., J Stat Phys (2012)
Esposito et al., Europhys Let (2010)
Diana, Bagci & Esposito, PRE (2013)

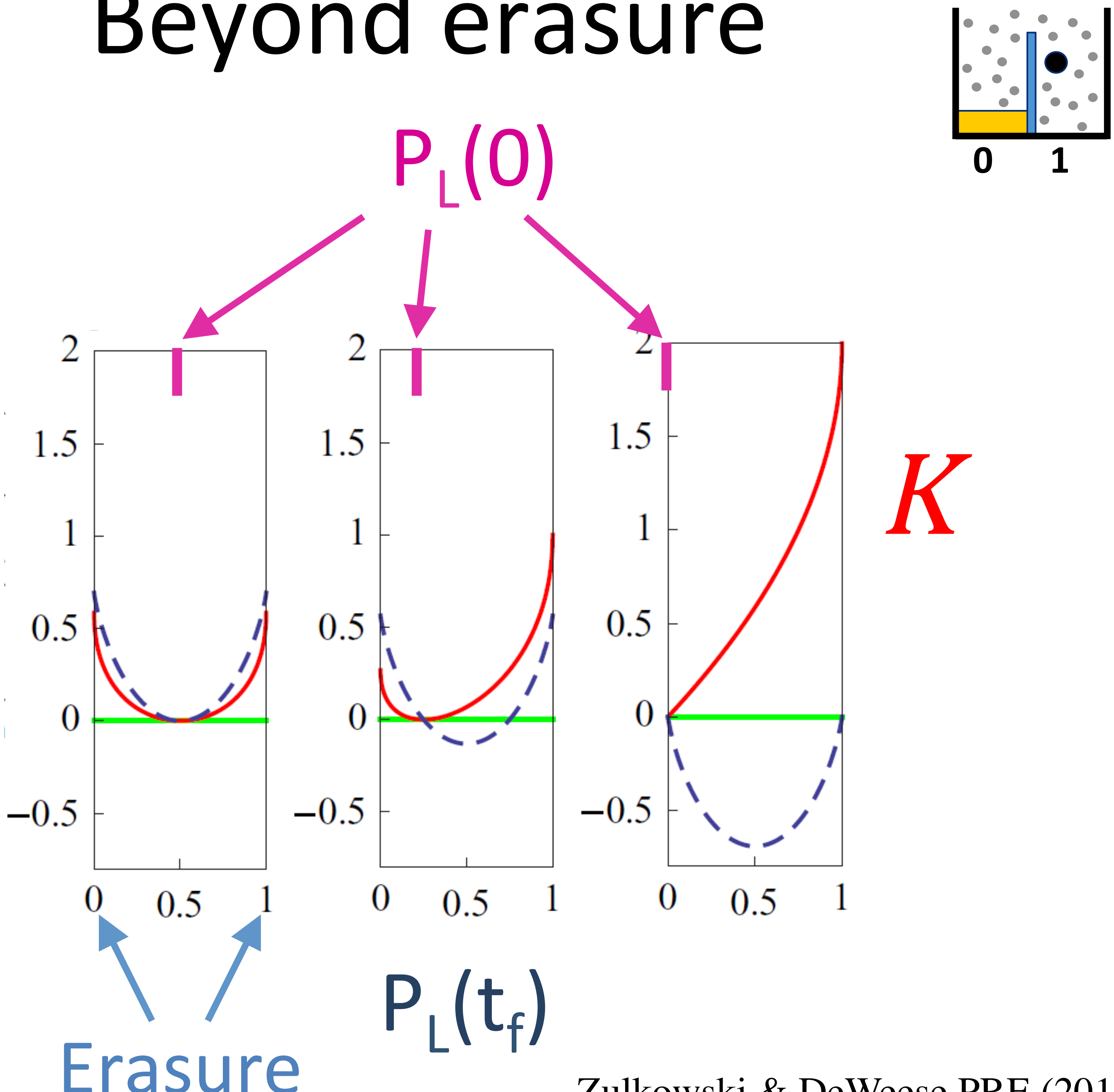
$$K \equiv [\sqrt{p_r(t_f)} - \sqrt{p_r(0)}]^2 + [\sqrt{p_l(t_f)} - \sqrt{p_l(0)}]^2$$

(K is twice the square of the Hellinger Distance)

$$\bar{t} \equiv \frac{2D}{l^2} t$$

Zulkowski & DeWeese PRE (2014)

Beyond erasure



Zulkowski & DeWeese PRE (2014)

New generalization from Slow Perturbation Theory

Time Dependent Fokker-Planck Equation

$$\frac{\partial}{\partial t}\rho(\mathbf{x};t) = \hat{\mathcal{L}}_{\boldsymbol{\lambda}(t)}(\mathbf{x})\rho(\mathbf{x};t)$$

Foker-Planck operator

$$\rho = \rho^{eq}$$

$$\langle \dot{Q} \rangle = 0$$

$$+ \frac{1}{\beta}\Delta S^{eq}$$

1st correction to equil. dist.

$$+ \int dt \boxed{\int dx' dx''\, \rho^{eq}_{\lambda(t)}(x'') \left[\partial_t \log \rho^{eq}_{\lambda(t)}(x'')\right] g_{\lambda(t)}\,(x''; x') \left[\partial_t \log \rho^{eq}_{\lambda(t)}(x')\right]}$$

$$+ \ldots$$

Explicit terms to all orders

Metric Tensor

Wadia, Zarcone, DeWeese, Mandal, in prep.

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