Introduction to Stochastic Thermodynamics: from Fluctuation Theorems to Thermodynamic Trade-off Relations

Lecture 4

2022 ICTP-KIAS School on Statistical Physics for Life Sciences

October 31- November 7, 2022

Jae Sung Lee

Korea Institute for Advanced Study

imagine the impossible

KIAS KOREA INSTITUTE FOR ADVANCED STUDY

2. TUR (Thermodynamic Uncertainty Relations) Lecture 3

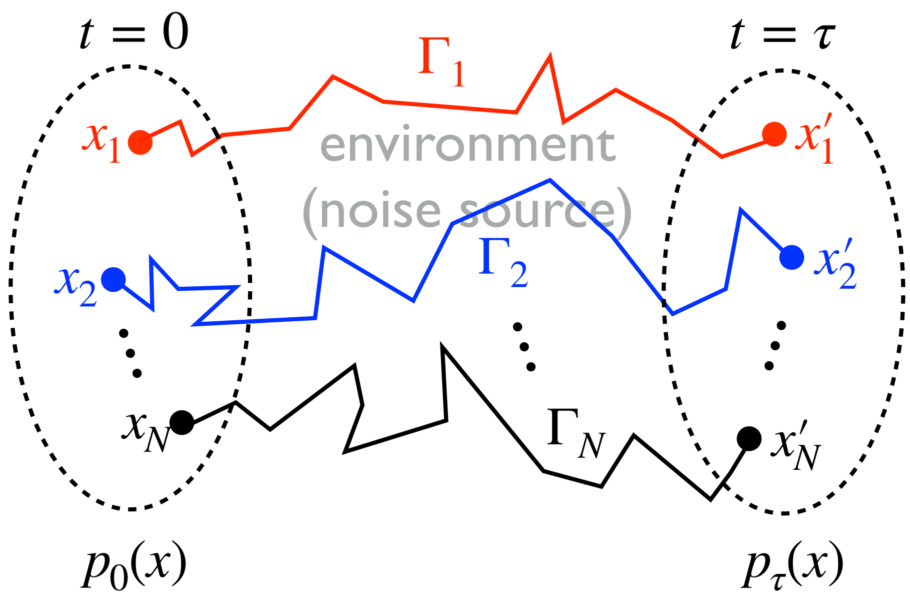
: relation of EP and fluctuation of Θ

$$\frac{\mathrm{Var}[\Theta]}{\langle\Theta\rangle^2}\langle\Sigma\rangle \geq 2k_\mathrm{B} \qquad \mathrm{Var}[\Theta] = \langle\Theta^2\rangle - \langle\Theta\rangle^2$$

$$\frac{\mathrm{Var}[X_\tau]}{\langle X_\tau\rangle^2}\downarrow \quad \langle\Sigma\rangle\uparrow \qquad\qquad \frac{\mathrm{Var}[X_\tau]}{\langle X_\tau\rangle^2}\uparrow \quad \langle\Sigma\rangle\downarrow$$

trade-off relation: we have to pay thermodynamic cost for reducing fluctuation

Schematic of a stochastic system



observable: $\Theta = \Theta(\Gamma)$ heat, work, displacement …

entropy production (EP): $\Sigma = \Sigma(\Gamma)$

3. Thermodynamic Speed Limit

: relation of EP and distribution

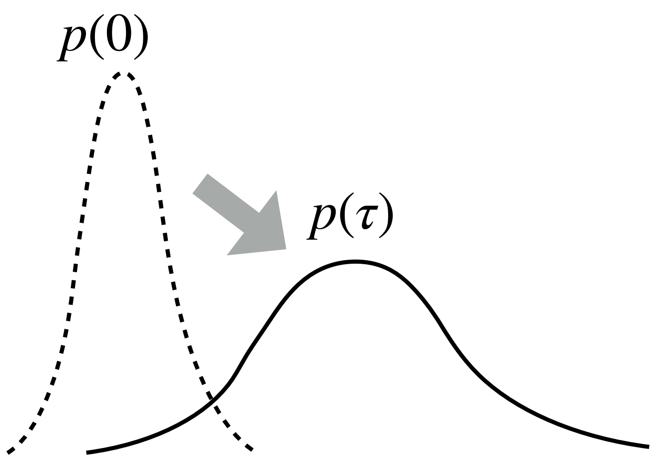
$$\tau\langle\Sigma\rangle \geq \frac{2d_{\mathrm{TV}}^2(p(0),p(\tau))}{\bar{A}} \quad \Rightarrow \quad \tau \geq \frac{2d_{\mathrm{TV}}^2(p(0),p(\tau))}{\langle\Sigma\rangle\bar{A}}$$

$d_{\mathrm{TV}}(p,q)$: distance between p and q

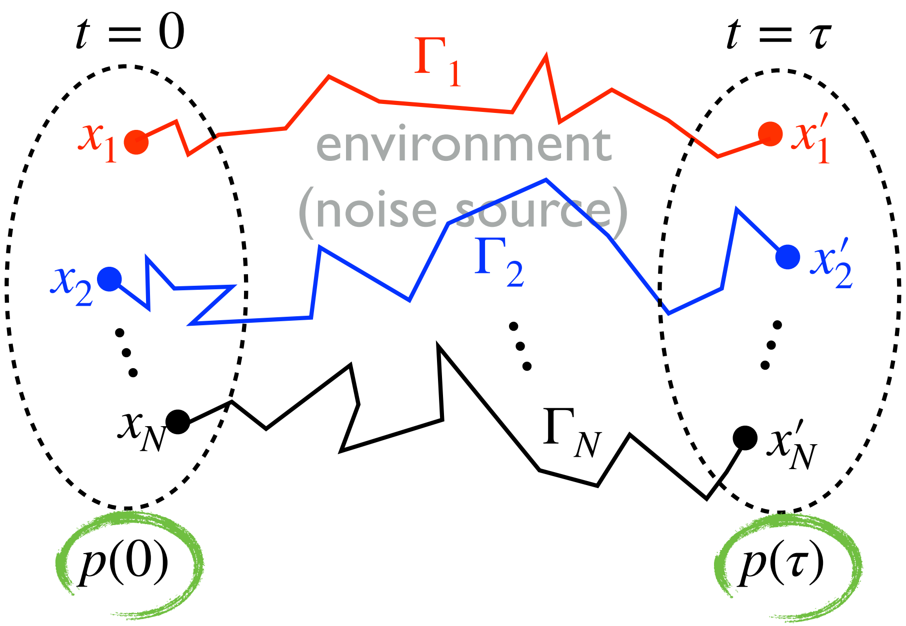
$\bar{A}$: dynamical activity (number of transitions)

$\tau \downarrow \quad \langle\Sigma\rangle \uparrow \qquad\qquad \tau \uparrow \quad \langle\Sigma\rangle \downarrow$

trade-off relation: we have to pay more thermodynamic cost for faster transition



Schematic of a stochastic system



observable: $\Theta = \Theta(\Gamma)$ heat, work, displacement …

entropy production (EP): $\Sigma = \Sigma(\Gamma)$

Contents of Lecture 4

1. Derivation of thermodynamic speed limit

2. Application of thermodynamic speed limit: finite-time Landauer's bound

Thermodynamic Speed Limit

: relation of EP and distribution

$$\tau\langle\Sigma\rangle \geq \frac{2d_{\mathrm{TV}}^2(p(0),p(\tau))}{\bar{A}} \;\Rightarrow\; \tau \geq \frac{2d_{\mathrm{TV}}^2(p(0),p(\tau))}{\langle\Sigma\rangle\bar{A}}$$

$d_{\mathrm{TV}}(p,q)$: distance between p and q

$\bar{A}$: dynamical activity (number of transitions)

c.f. Quantum speed limit Mandelstam / Tamm (1945)

closed quantum system: $\rho(0) \to \rho(\tau)$

classical limit : $\hbar \to 0$

$$\tau \geq \tau_{\mathrm{QSL}} \equiv \frac{\hbar\mathscr{L}(\rho(0),\rho(\tau))}{\Delta E} \;\longrightarrow\; \tau \geq \tau_{\mathrm{QSL}} = 0??$$

$$\mathscr{L}(\rho(0),\rho(\tau)) = \cos^{-1}(\sqrt{F(\rho(0),\rho(\tau))})$$

$$F(\rho(0),\rho(\tau)) \equiv \mathrm{tr}^2\left[\sqrt{\sqrt{\rho(0)}\rho(\tau)\sqrt{\rho(0)}}\right]$$

Thermodynamic Speed Limit

$$\tau \geq \frac{2d_{\mathrm{TV}}^2(p(0), p(\tau))}{\langle \Sigma \rangle \bar{A}} \quad \Rightarrow \ell \equiv d_{\mathrm{TV}}(p(0), p(\tau)) \qquad \tau \geq \frac{2\ell^2}{\langle \Sigma \rangle \bar{A}}$$

System setup: jump process with discrete states

$$\dot{p}_n(t) = \sum_{m(\neq n)} \left[R_{nm}(t) p_m(t) - R_{mn}(t) p_n(t) \right]$$

$p_n(t)$: probability of state n at t

$R_{nm}(t)$: $m \to n$ transition rate at t

$$\langle \dot{\Sigma} \rangle(t) = \sum_{m \neq n} R_{nm}(t) p_m(t) \ln \frac{R_{nm}(t) p_m(t)}{R_{mn}(t) p_n(t)}$$

$$\dot{A}(t) = \sum_{m \neq n} R_{nm}(t) p_m$$

$\dot{A}(t)$: dynamical activity (number of jumps) rate

$A(\tau) = \int_0^\tau \dot{A}(t) dt$: total number of jumps (total activity)

$\bar{A} = A(\tau)/\tau$: mean activity

$$d_{\mathrm{TV}}(p, q) = \frac{1}{2} \sum_n |p_n - q_n|$$

$0 \leq d_{\mathrm{TV}}(p, q) \leq 1$: total variation distance

General Form of Speed Limit

$$\tau \geq \frac{2\ell^2}{\langle \Sigma \rangle \bar{A}}$$

Shiraishi, Fun, Saito, PRL 121, 070601 (2018)
Vo, Vu, Hasegawa, PRE 102, 062132 (2020)

$$h\left(\frac{\ell}{A(\tau)}\right) \leq \frac{\langle \Sigma \rangle}{A(\tau)}$$

: key relation (convex function h exists)

↓

$$\frac{h\left(\frac{\ell}{A(\tau)}\right)}{2\frac{\ell}{A(\tau)}} \leq \frac{\frac{\langle \Sigma \rangle}{A(\tau)}}{2\frac{\ell}{A(\tau)}}$$

$$g(x) \equiv \frac{h(x)}{2x}$$

↓

$$\frac{\ell}{A(\tau)} \leq g^{-1}\left(\frac{\langle \Sigma \rangle}{2\ell}\right)$$

$$A(\tau) = \tau \bar{A}$$

↓

$$\tau \geq \frac{\ell}{\bar{A} g^{-1}\left(\frac{\langle \Sigma \rangle}{2\ell}\right)}$$

: general form

JSL, Lee, Kwon, Park, PRL 129, 120603 (2022)

General Form of Speed Limit

Derivation of $h\left(\frac{\ell}{A(\tau)}\right) \leq \frac{\langle \Sigma \rangle}{A(\tau)}$ JSL, Lee, Kwon, Park, PRL 129, 120603 (2022)

$$\ell = \frac{1}{2}\sum_n |p_n(0) - p_n(\tau)|$$

$$= \frac{1}{2}\sum_n \left| \int_0^\tau dt\ \dot{p}_n(t) \right|$$

$$\leq \frac{1}{2}\sum_n \int_0^\tau dt \left| \dot{p}_n(t) \right| \quad \leftarrow \quad \dot{p}_n(t) = \sum_{m(\neq n)} \left[R_{nm}(t) p_m(t) - R_{mn}(t) p_n(t) \right]$$

$$= \frac{1}{2}\sum_n \int_0^\tau dt \left| \sum_{m(\neq n)} \left[R_{nm}(t) p_m(t) - \sum_{m(\neq n)} R_{mn}(t) p_n(t) \right] \right|$$

$$\leq \frac{1}{2}\int_0^\tau dt \sum_{n\neq m} \left| R_{nm}(t) p_m(t) - R_{mn}(t) p_n(t) \right|$$

General Form of Speed Limit

Derivation of $h\left(\frac{\ell}{A(\tau)}\right) \le \frac{\langle\Sigma\rangle}{A(\tau)}$ JSL, Lee, Kwon, Park, PRL 129, 120603 (2022)

$$\ell = \frac{1}{2}\sum_n |p_n(0) - p_n(\tau)|$$

$$\le \frac{1}{2}\int_0^\tau dt \sum_{n\neq m} \left| R_{nm}(t)p_m(t) - R_{mn}(t)p_n(t) \right| = \frac{1}{2}\int_0^\tau dt\ \dot{A}(t) \sum_{n\neq m} \left| Q_{nm} - Q^*_{nm} \right|$$

$$Q_{nm} = \frac{R_{nm}(t)p_m(t)}{\dot{A}(t)} \qquad Q^*_{nm} = \frac{R_{mn}(t)p_n(t)}{\dot{A}(t)} \qquad \dot{A}(t) = \sum_{m\neq n} R_{nm}(t)p_m$$

probability normalization

$$\to \frac{1}{2}\sum_{n\neq m} \left| Q_{nm} - Q^*_{nm} \right| = d_{\mathrm{TV}}(Q, Q^*)$$

$$= \int_0^\tau dt\ \dot{A}(t) d_{\mathrm{TV}}(Q, Q^*)$$

General Form of Speed Limit

Derivation of $h\left(\frac{\ell}{A(\tau)}\right) \le \frac{\langle\Sigma\rangle}{A(\tau)}$ JSL, Lee, Kwon, Park, PRL 129, 120603 (2022)

$$Q_{nm} = \frac{R_{nm}(t)p_m(t)}{\dot{A}(t)} \qquad Q^*_{nm} = \frac{R_{mn}(t)p_n(t)}{\dot{A}(t)}$$

$$\ell = \frac{1}{2}\sum_n |p_n(0) - p_n(\tau)|$$

$$\le \frac{1}{2}\int_0^\tau dt \sum_{n\neq m} \left| R_{nm}(t)p_m(t) - R_{mn}(t)p_n(t) \right| = \frac{1}{2}\int_0^\tau dt\ \dot{A}(t) \sum_{n\neq m} \left| Q_{nm} - Q^*_{nm} \right|$$

$$= \int_0^\tau dt\ \dot{A}(t) d_{\mathrm{TV}}(Q, Q^*) \le \int_0^\tau dt\ \dot{A}(t) h^{-1}\left(D(Q\|Q^*)\right) = \int_0^\tau dt\ \dot{A}(t) h^{-1}\left(\frac{\langle\dot{\Sigma}\rangle(t)}{\dot{A}(t)}\right)$$

$$= A(\tau)\int_0^\tau dt\ \frac{\dot{A}(t)}{A(\tau)} h^{-1}\left(\frac{\langle\dot{\Sigma}\rangle(t)}{\dot{A}(t)}\right)$$

$$\le A(\tau) h^{-1}\left(\int_0^\tau dt\ \frac{\dot{A}(t)}{A(\tau)}\frac{\langle\dot{\Sigma}\rangle(t)}{\dot{A}(t)}\right)$$

Jesen (concavity)

$$= A(\tau) h^{-1}\left(\frac{\langle\Sigma\rangle}{A(\tau)}\right)$$

$$D(Q\|Q^*) = \sum_{n\neq m} \frac{R_{nm}p_m}{\dot{A}(t)} \ln \frac{R_{nm}p_m}{R_{mn}p_n} = \frac{\langle\dot{\Sigma}\rangle(t)}{\dot{A}(t)}$$

Statistical distances and their relation

total variation distance

$$d_{\mathrm{TV}}(p, q) = \frac{1}{2}\sum_n |p_n - q_n| \qquad 0 \le d_{\mathrm{TV}}(p, q) \le 1$$

Kullback-Leibler (KL) divergence

$$D(p\|q) = \sum_n p_n \ln \frac{p_n}{q_n} \qquad 0 \le D(p\|q)$$

convex function h

$$h\left(d_{\mathrm{TV}}(p, q)\right) \le D(p\|q)$$

General Form of Speed Limit

Derivation of $h\left(\frac{\ell}{A(\tau)}\right) \le \frac{\langle\Sigma\rangle}{A(\tau)}$

JSL, Lee, Kwon, Park, PRL 129, 120603 (2022)

$$\ell = \frac{1}{2}\sum_n |p_n(0) - p_n(\tau)|$$

$$\le A(\tau) h^{-1}\left(\frac{\langle\Sigma\rangle}{A(\tau)}\right)$$

$$Q_{nm} = \frac{R_{nm}(t)p_m(t)}{\dot{A}(t)} \qquad Q^*_{nm} = \frac{R_{mn}(t)p_n(t)}{\dot{A}(t)}$$

$$D(Q\|Q^*) = \sum_{n\neq m} \frac{R_{nm}p_m}{\dot{A}(t)} \ln \frac{R_{nm}p_m}{R_{mn}p_n} = \frac{\langle\dot{\Sigma}\rangle(t)}{\dot{A}(t)}$$

$$= \sum_{m\neq n} \frac{R_{mn}p_n}{\dot{A}(t)} \ln \frac{R_{mn}p_n}{R_{nm}p_m} = D(Q^*\|Q)$$

$\rightarrow \; D(Q\|Q^*) = D(Q^*\|Q)$

symmetric Kullback-Leibler divergence (KLD)

General Form of Speed Limit

$$\tau \geq \frac{\ell}{\bar{A} g^{-1}\left(\frac{\langle \Sigma \rangle}{2\ell}\right)} \qquad g(x) \equiv \frac{h(x)}{2x}$$

: general form

JSL, Lee, Kwon, Park, PRL 129, 120603 (2022)

Statistical distances and their relation

convex function h

$$h\left(d_{\mathrm{TV}}(p,q)\right) \leq D(p\|q)$$

$h(x) = 2x^2$ [Pinsker (1960)]

$= -\ln(1-x^2)$ [Bretagnolle-Huber (1979)]

$= \ln\left[(1+x)^{-1+x}/(1-x)\right]$ [Gilardoni (2008)]

if $D(p\|q) = D(q\|p)$

$= x\ln\left[(1+x)/(1-x)\right]$ [Gilardoni (2008)]

(tightest)

$D(Q\|Q^*) = D(Q^*\|Q)$: symmetric KLD

$0 \leq d_{\mathrm{TV}}(p,q) \leq 1 \qquad 0 \leq D(p\|q)$

$p = (p_1, p_2) = (0,1)$

$q = (q_1, q_2) = (1,0)$

$\Rightarrow$

$d_{\mathrm{TV}} = 1 \leftarrow \frac{1}{2}(|1-0| + |0-1|)$

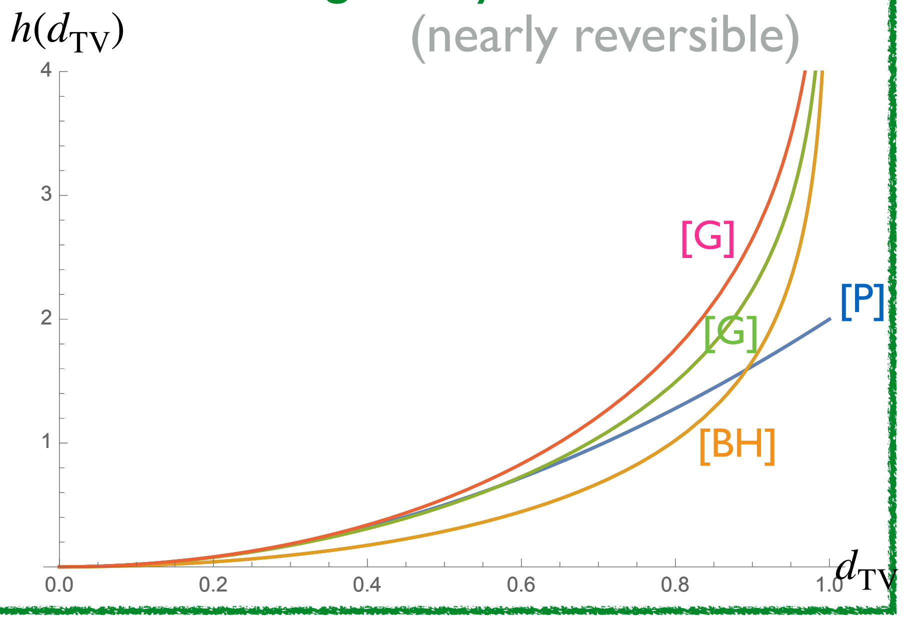
$D(p\|q) = \infty \leftarrow 1\ln(1/0) + 0\ln(0/1)$

Pinsker is very loose near $d_{\mathrm{TV}} = 1$.

(highly irreversible)

is tight only when $d_{\mathrm{TV}} \approx 0$.

(nearly reversible)



General Form of Speed Limit

$$\tau \geq \frac{\ell}{\bar{A} g^{-1}\left(\frac{\langle\Sigma\rangle}{2\ell}\right)} \qquad g(x) \equiv \frac{h(x)}{2x}$$

: general form

JSL, Lee, Kwon, Park, PRL 129, 120603 (2022)

Statistical distances and their relation

convex function h

$$h\left(d_{\mathrm{TV}}(p,q)\right) \leq D(p\|q)$$

$$h(x) = 2x^2$$ [Pinsker (1960)] → $$\tau \geq \frac{2\ell^2}{\langle\Sigma\rangle \bar{A}}$$ (previous)

$$= -\ln(1-x^2)$$ [Bretagnolle-Huber (1979)]

tight for nearly reversible

loose for highly irreversible

$$= \ln\left[(1+x)^{-1+x}/(1-x)\right]$$ [Gilardoni (2008)]

(symmetric KLD bound)

if $D(p\|q) = D(q\|p)$

$$= x \ln\left[(1+x)/(1-x)\right]$$ [Gilardoni (2008)] (tightest) → $$\tau \geq \frac{\ell}{\bar{A}\tanh\left(\langle\Sigma\rangle/(2\ell)\right)}$$ (tightest)

tight for all processes

$D(Q\|Q^*) = D(Q^*\|Q)$: symmetric KLD

Derivation of the Tightest Symmetric KLD Bound

if $D(p\|q) = D(q\|p) \longrightarrow h(x) = x \ln\left[(1+x)/(1-x)\right]$

$$d_{\mathrm{TV}}(p,q)^2 = \left(\frac{1}{2}\sum_n |p_n - q_n|\right)^2 = \left(\frac{1}{2}\sum_n \frac{|p_n - q_n|}{\sqrt{p_n + q_n}} \cdot \sqrt{p_n + q_n}\right)^2$$

$$\le \frac{1}{4}\sum_n \frac{|p_n - q_n|^2}{p_n + q_n} \cdot \underbrace{\sum_n (p_n + q_n)}_{=2} = \frac{1}{2}\sum_n \frac{|p_n - q_n|^2}{p_n + q_n} \equiv d_{\mathrm{LC}}(p,q)^2$$

Cauchy-Schwarz

Le Cam distance

$$d_{\mathrm{LC}}(p,q)^2 = d_{\mathrm{TV}}(p,q) \sum_n \underbrace{\frac{|p_n - q_n|}{2 d_{\mathrm{TV}}(p,q)}}_{\equiv \tilde{p}_n} \cdot \underbrace{\frac{|p_n - q_n|}{p_n + q_n}}_{} = \tanh\left|\frac{1}{2}\ln\frac{p_n}{q_n}\right|$$

$$\le d_{\mathrm{TV}}(p,q) \tanh\left(\sum_n \tilde{p}_n \left|\frac{1}{2}\ln\frac{p_n}{q_n}\right|\right)$$

concavity of tanh

$$= d_{\mathrm{TV}}(p,q) \tanh\left[\frac{1}{4 d_{\mathrm{TV}}(p,q)} \sum_n (p_n - q_n)\ln\frac{p_n}{q_n}\right] = d_{\mathrm{TV}}(p,q) \tanh\left[\frac{D_{\mathrm{S}}(p\|q)}{2 d_{\mathrm{TV}}(p,q)}\right]$$

$$\tanh^{-1} x = \frac{1}{2}\ln\frac{1+x}{1-x}$$

$$\frac{1}{2}\sum_n (p_n - q_n)\ln\frac{p_n}{q_n} = \frac{1}{2}\left[D(p\|q) + D(q\|p)\right] \equiv D_{\mathrm{S}}(p\|q)$$

$\rightarrow d_{\mathrm{TV}}(p,q) \le \tanh[D_{\mathrm{S}}(p\|q)/2 d_{\mathrm{TV}}(p,q)]$

if $D(p\|q) = D(q\|p)$, $D_{\mathrm{S}}(p\|q) = D(p\|q)$

$\therefore 2 d_{\mathrm{TV}}(p,q) \tanh^{-1} d_{\mathrm{TV}}(p,q) \le D_{\mathrm{S}}(p\|q)$

$\rightarrow h\left(2 d_{\mathrm{TV}}(p,q)\right) \le D(p\|q)$

Application to Finite-Time Landauer's Bound

Landauer's bound

For erasing one bit of information, at least $k_{\mathrm{B}}T \ln 2$ should be dissipated.

$\rightarrow Q \geq k_{\mathrm{B}}T \ln 2$

This minimum bound is attained in the quasi-static limit.

For finite-time process,

$\rightarrow Q \geq k_{\mathrm{B}}T \ln 2 +$ additional cost

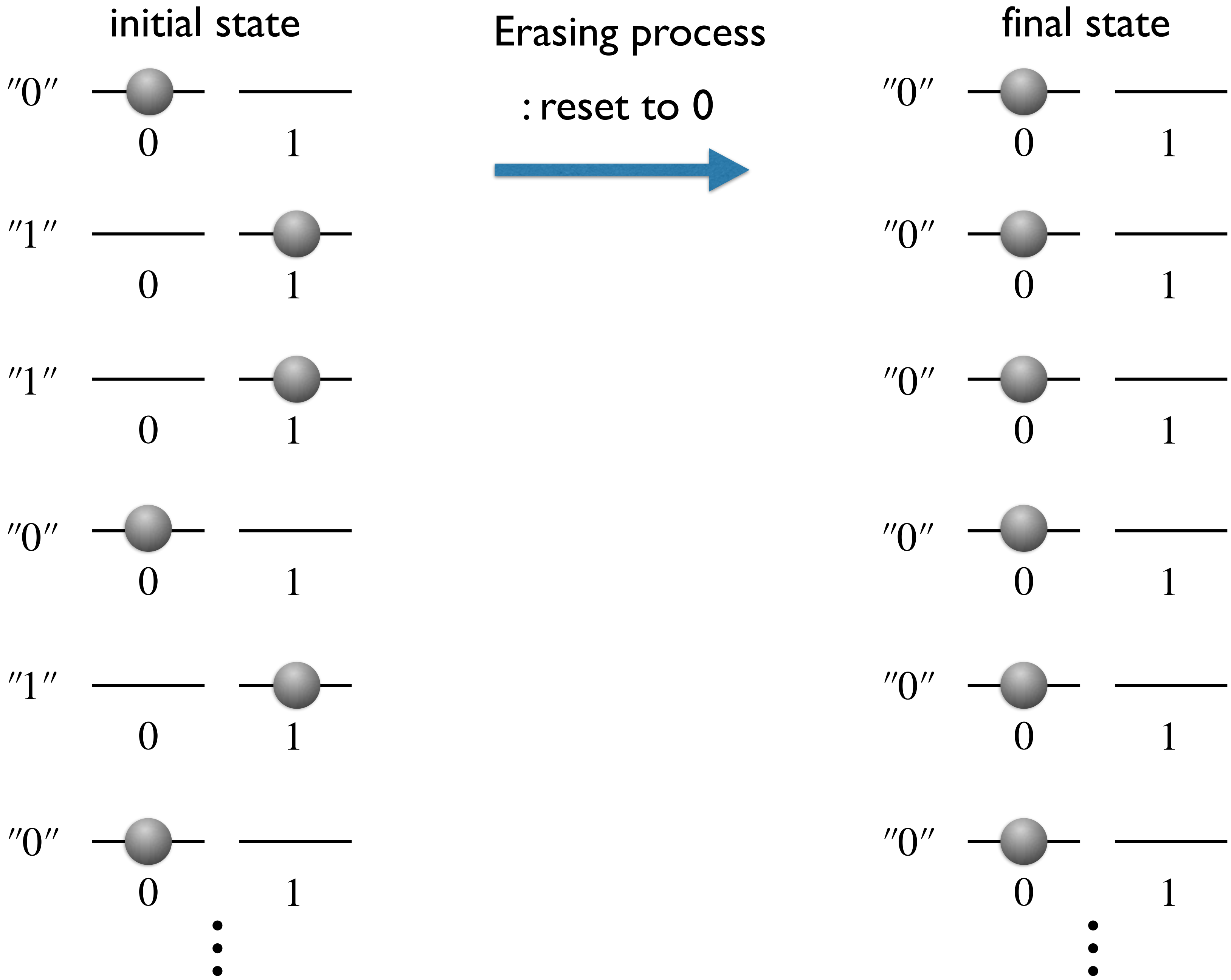
double-well potential: $\sim \dfrac{1}{\tau}$

[exp] Berut et al., Nature 483, 187-189 (2012)

[exp] Jun, Gavrilov, Bechhoefer, PRL 113, 190601 (2014)

[theory] Proesmans, Ehrich, and Bechhoefer PRL 125, 100602 (2020), PRE 102, 032105 (2020)

Application to Finite-Time Landauer's Bound



$p_0(0) = \frac{1}{2}$ $\quad p_1(0) = \frac{1}{2}$

$p_0(\tau) = 1$ $\quad p_1(\tau) = 0$

Application to Finite-Time Landauer's Bound

Erasing process

initial state

$$p_0(0) = \frac{1}{2} \quad p_1(0) = \frac{1}{2}$$

final state

$$p_0(\tau) = 1 \quad p_1(\tau) = 0$$

total variation distance: $\ell = d_\mathrm{T}\left(p(0), p(\tau)\right) = \sum_{n=0}^{1} |p_n(0) - p_n(\tau)| = \frac{1}{2}$

Shannon EP change: $\Delta S_\mathrm{sys}/k_\mathrm{B} = \sum_n p_n(0) \ln p_n(0) - \sum_n p_n(\tau) \ln p_n(\tau) = -\ln 2$

speed limit

$$\tau \geq \frac{\ell}{\bar{A} g^{-1}\left(\frac{\langle \Sigma \rangle}{2\ell}\right)} \Rightarrow \langle \Sigma \rangle \geq 2\ell g(v)$$

where $v \equiv \frac{\ell}{A(\tau)}$

$$Q \geq k_\mathrm{B} T \ln 2 + 2T\ell g(v)$$

additional cost

$$\langle \Sigma \rangle = -k_\mathrm{B} \ln 2 + \frac{Q}{T}$$

Pinsker: $\frac{2T\ell^2}{\tau \bar{A}}$ previous $\sim \frac{1}{\tau}$ behavior

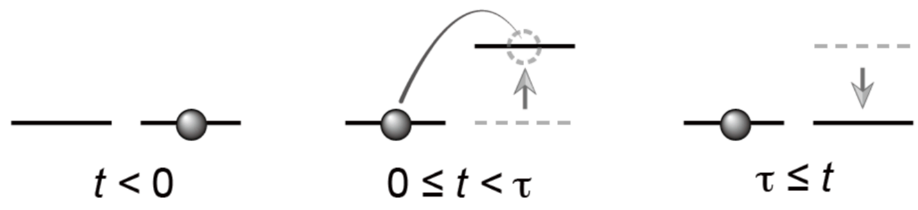
Zhen, et al., PRL 127, 190602 (2021)

symmetric KLD: $T\ell \ln\left(\frac{1+v}{1-v}\right)$ (tightest)

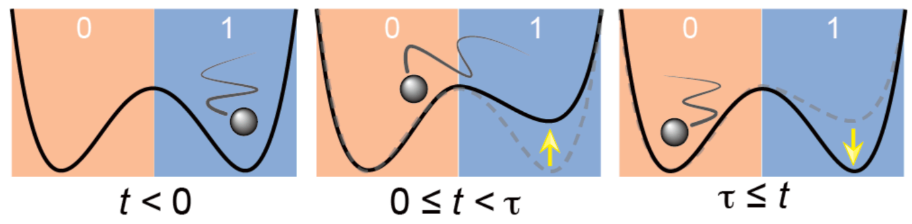
Application to Finite-Time Landauer's Bound

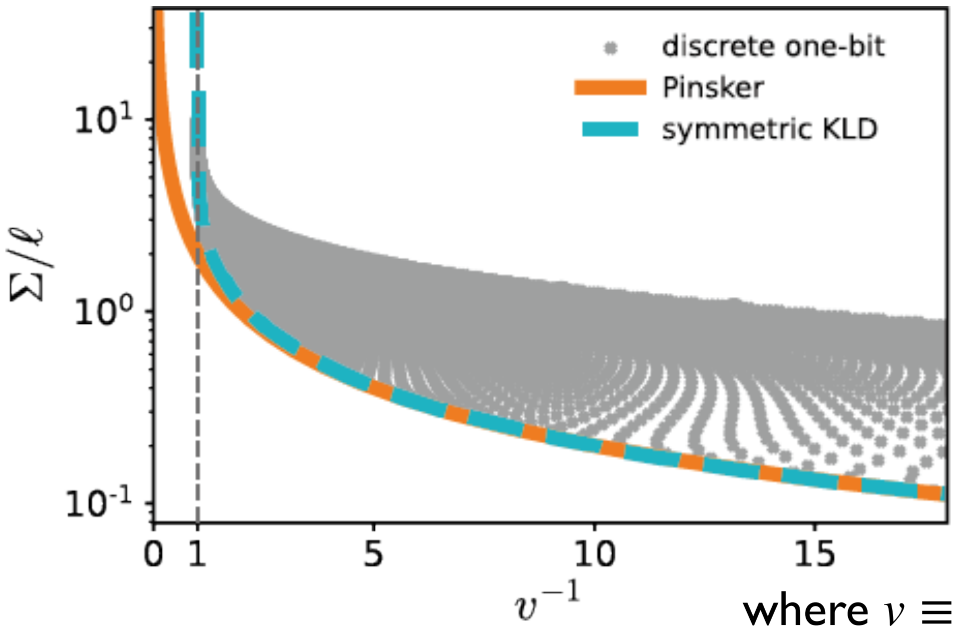
Model studies

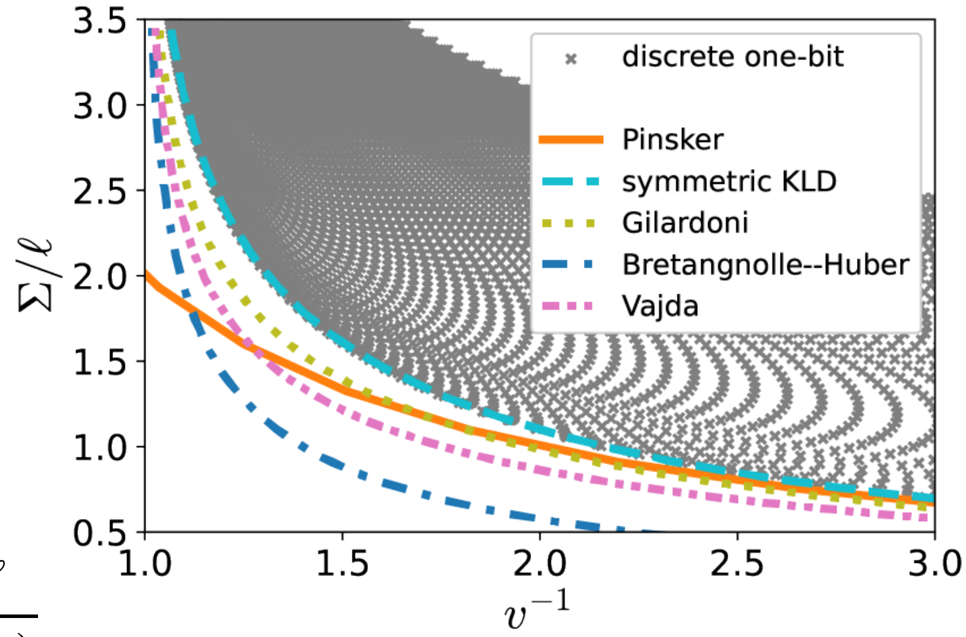
1. discrete one-bit model



2. coarse-grained bit model







where $v \equiv \dfrac{\ell}{A(\tau)}$

Pinsker: $\langle \Sigma \rangle / \ell \geq 2v$

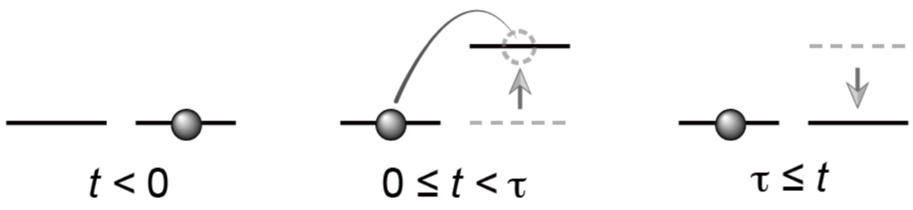
symmetric KLD: $\langle \Sigma \rangle / \ell \geq \ln \left(\dfrac{1+v}{1-v} \right)$

Pinsker is infinitely loose compared with the symmetric KLD near $v = 1$.

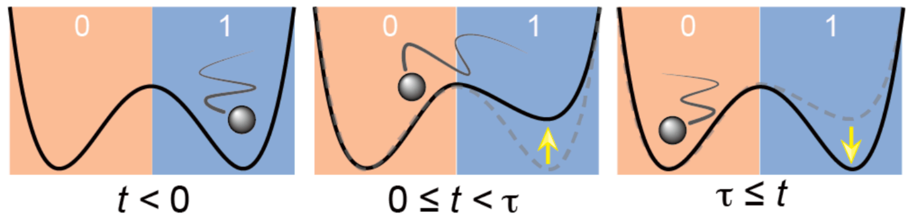
Application to Finite-Time Landauer's Bound

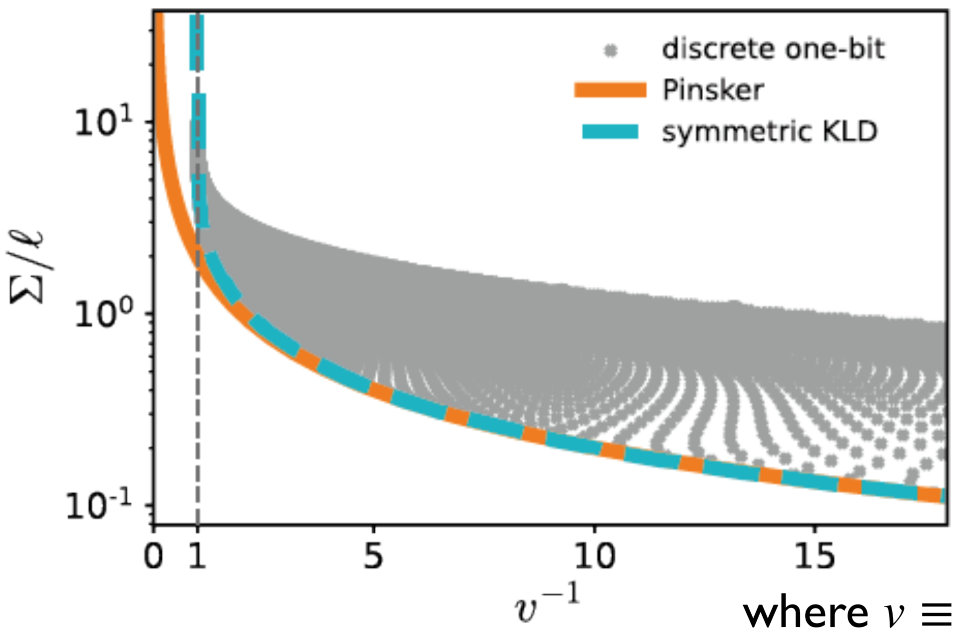
Model studies

1. discrete one-bit model

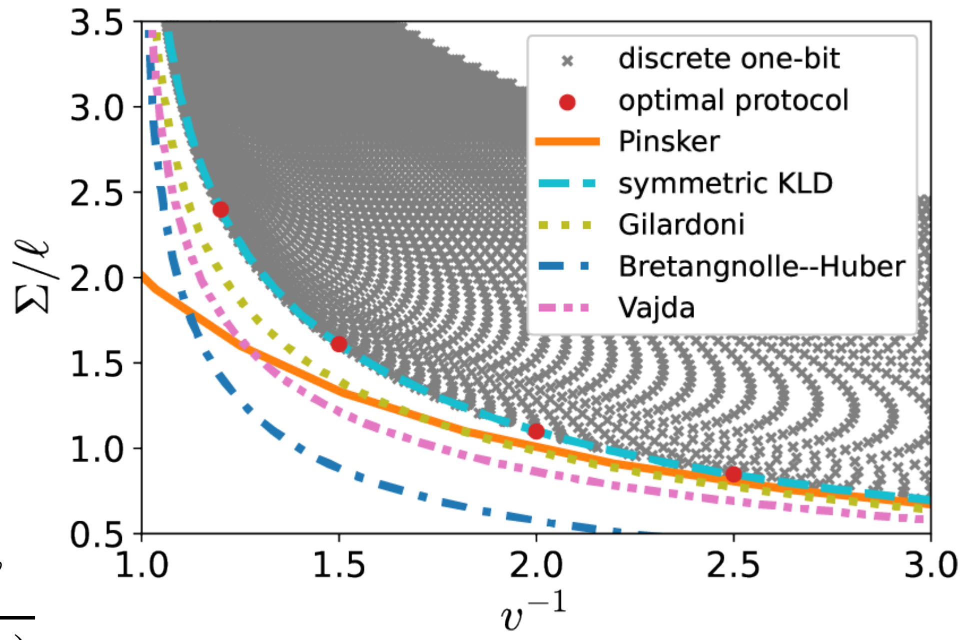


2. coarse-grained bit model





where $v \equiv \dfrac{\ell}{A(\tau)}$



Pinsker: $\langle \Sigma \rangle / \ell \geq 2v$

symmetric KLD: $\langle \Sigma \rangle / \ell \geq \ln \left(\dfrac{1+v}{1-v} \right)$

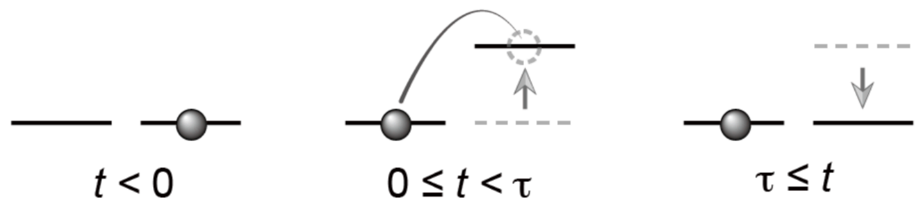
sufficient condition for optimal protocol

$$\frac{R_{01}(t)p_1(t)}{R_{10}(t)p_0(t)} = c \text{ (const.)}, \quad \forall\ 0 \leq t \leq \tau$$

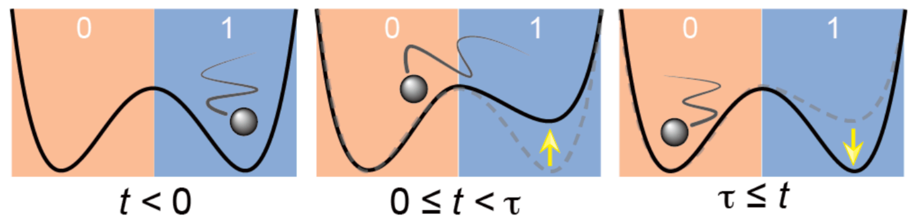
Application to Finite-Time Landauer's Bound

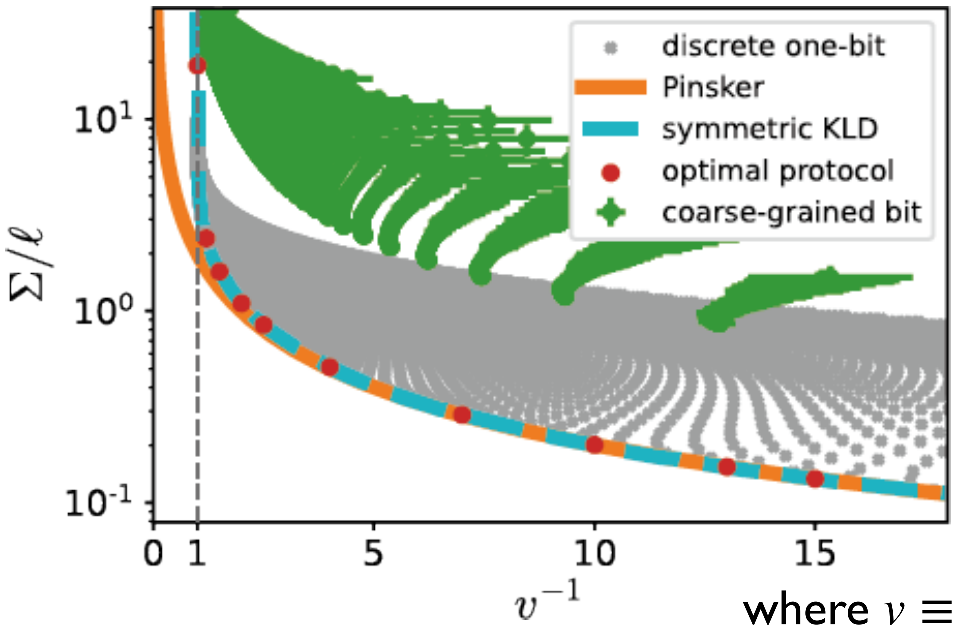
Model studies

1. discrete one-bit model

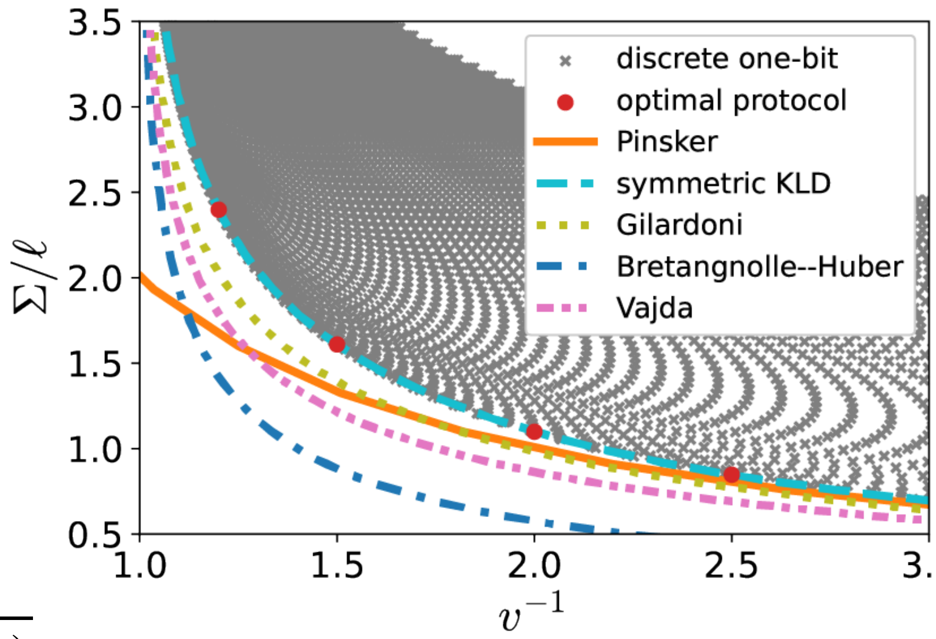


2. coarse-grained bit model





where $v \equiv \dfrac{\ell}{A(\tau)}$



Pinsker: $\langle\Sigma\rangle/\ell \geq 2v$

symmetric KLD: $\langle\Sigma\rangle/\ell \geq \ln\left(\dfrac{1+v}{1-v}\right)$

$$\langle\Sigma\rangle = \langle\Sigma\rangle^{\text{inter}} + \langle\Sigma\rangle^{\text{intra}}$$

where $v^{\text{cg}} \equiv \dfrac{\ell^{\text{cg}}}{A^{\text{cg}}(\tau)}$

$$\geq \langle\Sigma\rangle^{\text{inter}} \geq \langle\Sigma\rangle^{\text{cg}} \geq \ell^{\text{cg}} g(v^{\text{cg}})$$

Summary: Speed Limit

1. Speed Limit: trade-off between time and thermodynamic cost

2. General form of the speed limit

$$\tau \geq \frac{\ell}{\bar{A} g^{-1}\left(\frac{\langle \Sigma^* \rangle}{2\ell}\right)}$$

3. Application: tight finite-time Landauer's bound

$$Q \geq k_{\mathrm{B}} T \ln 2 + \underline{2T\ell g(v)}$$

additional cost

Pinsker: $\dfrac{2T\ell^2}{\tau \bar{A}}$ previous $\sim \dfrac{1}{\tau}$ behavior

symmetric KLD: $T\ell \ln\left(\dfrac{1+v}{1-v}\right)$ (tightest)