Introduction to

Stochastic Thermodynamics

Lecture 3

The 22nd KIAS-APCTP Winter School on Statistical Physics

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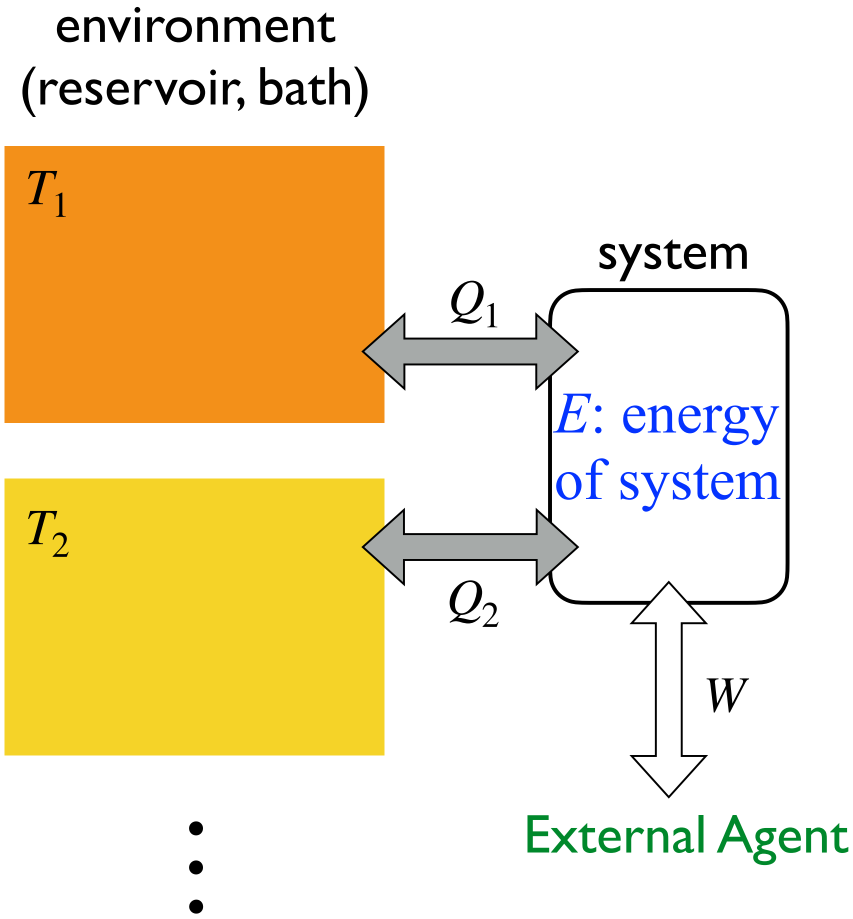
What is Thermodynamics?

a branch of physics that deals with **heat**, **work**, and **temperature**, and **their relation** to **energy**, **entropy**…

Wikipedia: Thermodynamics



heat: energy transfer btw system and bath

work: energy transfer btw system and E.A.

→ open system

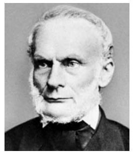
Relation for energy

$$1^{\mathrm{st}}: \quad \Delta E = Q_1 + Q_2 + W$$

Relation for entropy

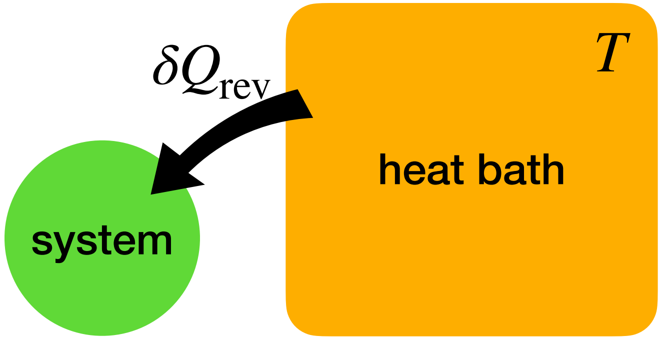
$$2^{\mathrm{nd}}: \quad \Delta S_{\mathrm{tot}} \geq 0$$

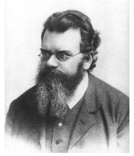
Entropy



Rudolf Clausius (1865): $dS_{\mathrm{sys}} = \dfrac{\delta Q_{\mathrm{rev}}}{T}$

thermodynamic definition

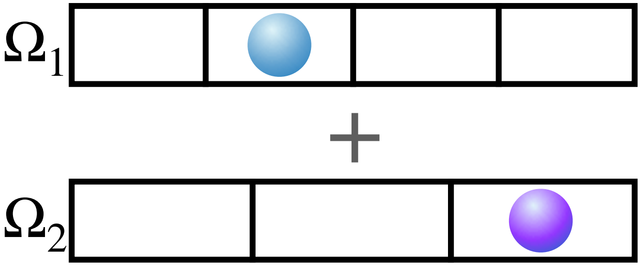




Ludwig Boltzmann (1877): $S = k_{\mathrm{B}} \ln \Omega$

statistical mechanics definition

Ω : # of state



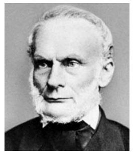
two independent systems

additivity: $S_1 = k_{\mathrm{B}} \ln \Omega_1$

$$S_2 = k_{\mathrm{B}} \ln \Omega_2$$

$$S = k_{\mathrm{B}} \ln(\Omega_1 \Omega_2) = S_1 + S_2$$

Entropy



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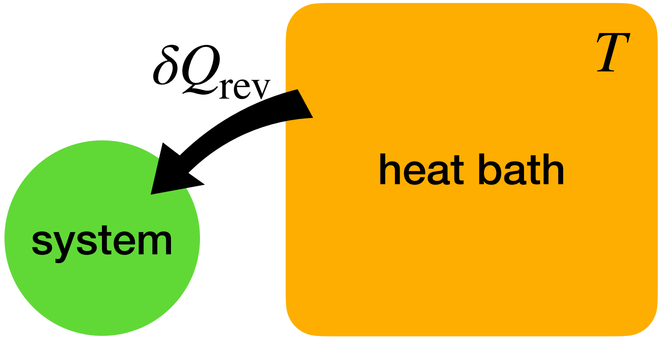

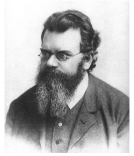

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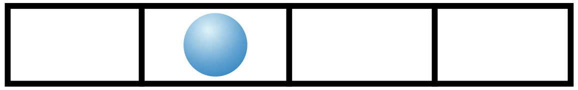
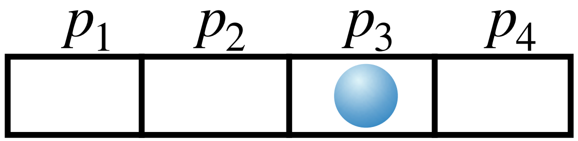
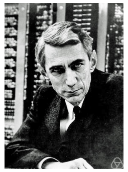


$$S = -k_B \sum_i p_i \ln p_i$$



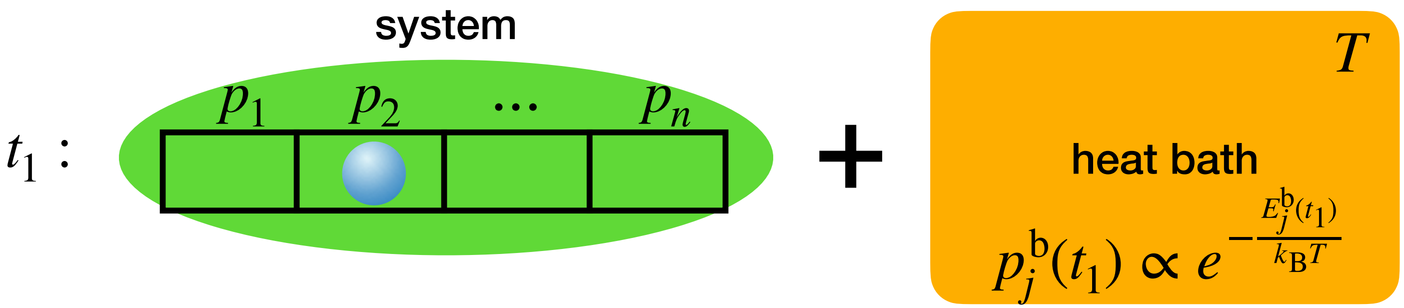
when $p_i = 1/\Omega$, $S = k_B \ln \Omega$



Claude Shannon (1948): $S = -\sum_i p_i \ln p_i$ (information, uncertainty)

In equilibrium, Clausius (thermodynamic) and Shannon (stat-mech) are identical.

Entropy Production



system

$t_1 :$

$p_1 \quad p_2 \quad \cdots \quad p_n$

$+$

T

heat bath

$p_j^{\mathrm{b}}(t_1) \propto e^{-\frac{E_j^{\mathrm{b}}(t_1)}{k_{\mathrm{B}}T}}$

Entropy : $S_{\mathrm{sys}}(t_1) = -k_{\mathrm{B}} \sum_i p_i(t_1) \ln p_i(t_1)$

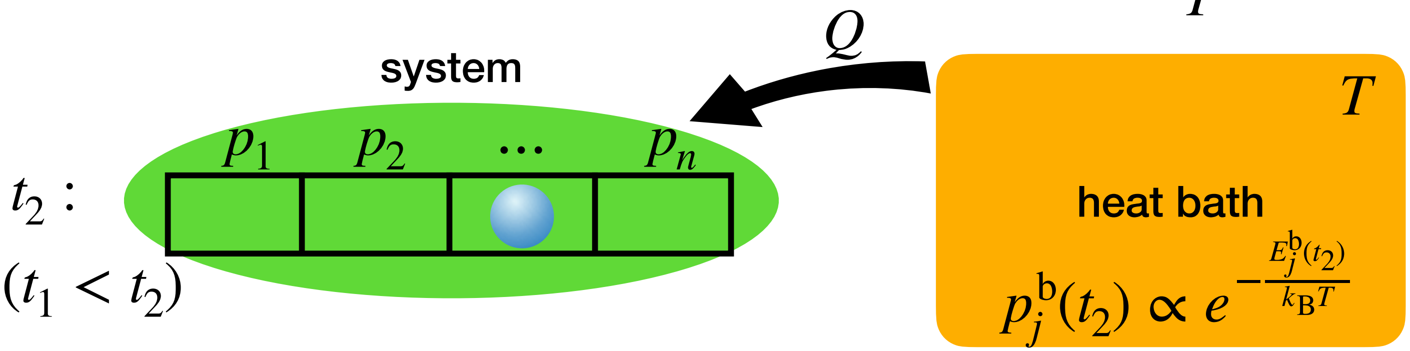
$$S_{\mathrm{b}}(t_1) = -k_{\mathrm{B}} \sum_j p_j^{\mathrm{b}}(t_1) \ln p_j^{\mathrm{b}}(t_1)$$

$$= \sum_j p_j^{\mathrm{b}}(t_1) E_j^{\mathrm{b}}(t_1)/T + c$$

$$= \frac{\langle E^{\mathrm{b}}(t_1) \rangle}{T} + c$$

(assume independence of system and bath)

$$S_{\mathrm{tot}}(t_1) = S_{\mathrm{sys}}(t_1) + S_{\mathrm{b}}(t_1)$$



system

$t_2 :$

$(t_1 < t_2)$

$p_1 \quad p_2 \quad \cdots \quad p_n$

Q

T

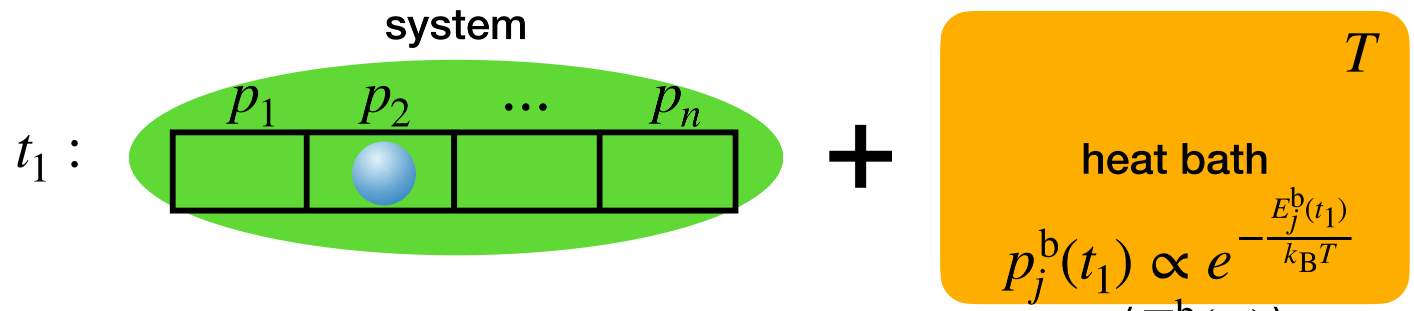
heat bath

$p_j^{\mathrm{b}}(t_2) \propto e^{-\frac{E_j^{\mathrm{b}}(t_2)}{k_{\mathrm{B}}T}}$

$$S_{\mathrm{tot}}(t_2) = S_{\mathrm{sys}}(t_2) + S_{\mathrm{b}}(t_2)$$

$$S_{\mathrm{sys}}(t_2) = -k_{\mathrm{B}} \sum_i p_i(t_2) \ln p_i(t_2) \qquad S_{\mathrm{b}}(t_2) = \frac{\langle E^{\mathrm{b}}(t_2) \rangle}{T} + c$$

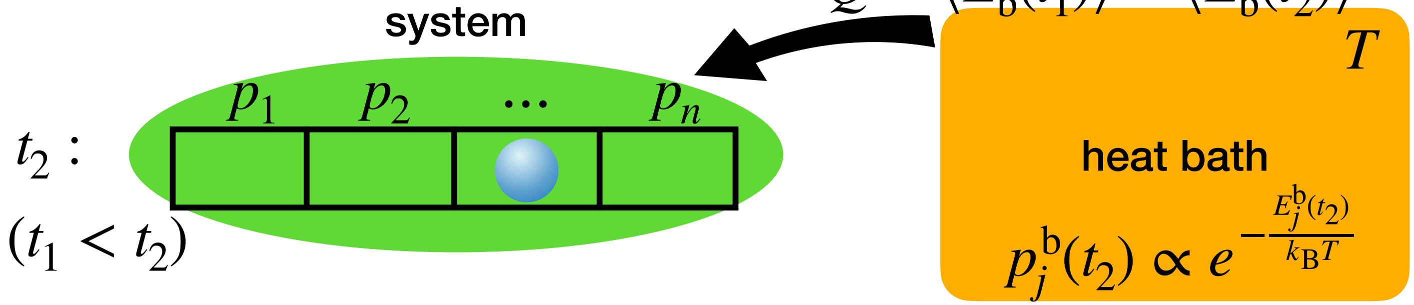
Entropy Production



Entropy : $S_{\mathrm{sys}}(t_1) = -k_{\mathrm{B}} \sum_i p_i(t_1) \ln p_i(t_1)$ $\qquad S_{\mathrm{b}}(t_1) = \dfrac{\langle E^{\mathrm{b}}(t_1) \rangle}{T} + c$

$$S_{\mathrm{tot}}(t_1) = S_{\mathrm{sys}}(t_1) + S_{\mathrm{b}}(t_1)$$

$$Q = \langle E_{\mathrm{b}}(t_1) \rangle - \langle E_{\mathrm{b}}(t_2) \rangle$$



$$S_{\mathrm{tot}}(t_2) = S_{\mathrm{sys}}(t_2) + S_{\mathrm{b}}(t_2)$$

$S_{\mathrm{sys}}(t_2) = -k_{\mathrm{B}} \sum_i p_i(t_2) \ln p_i(t_2)$ $\qquad S_{\mathrm{b}}(t_2) = \dfrac{\langle E^{\mathrm{b}}(t_2) \rangle}{T} + c$

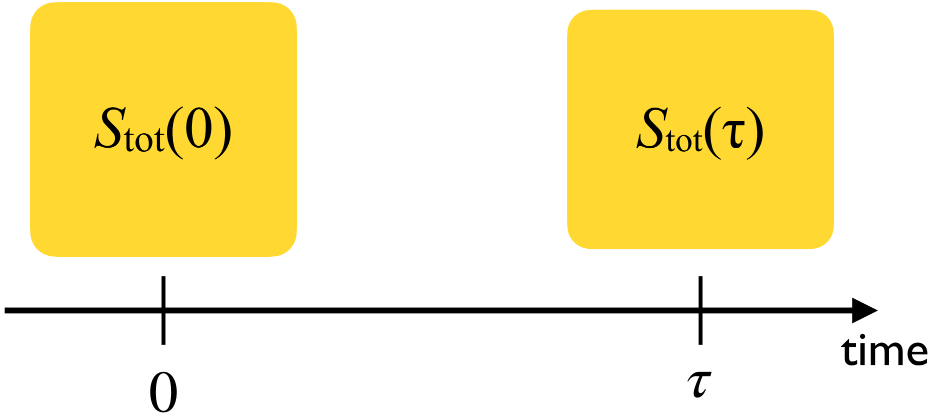
$$\Delta S_{\mathrm{tot}} = S_{\mathrm{tot}}(t_2) - S_{\mathrm{tot}}(t_1) = \Delta S_{\mathrm{sys}} + \Delta S_{\mathrm{b}}$$

$$= \Delta S_{\mathrm{sys}} - \frac{Q}{T}$$

$$\Delta S_{\mathrm{sys}} = S_{\mathrm{sys}}(t_2) - S_{\mathrm{sys}}(t_1)$$

$$\Delta S_{\mathrm{b}} = S_{\mathrm{b}}(t_2) - S_{\mathrm{b}}(t_1) = -\frac{Q}{T}$$

Thermodynamic Second Law

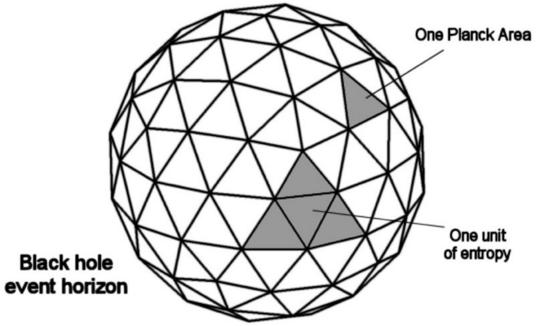


$$\Delta S_{\mathrm{tot}} = S_{\mathrm{tot}}(\tau) - S_{\mathrm{tot}}(0) \geq 0$$

$$(\Delta S_{\mathrm{tot}} = 0 \text{ when process is reversible})$$

Simple, but governing whole universe!

Black hole



$$S_{\mathrm{BH}} = \frac{c^3 A}{4G\hbar}$$

Quantum system

$$S(\rho) = -\operatorname{Tr}(\rho \ln \rho)$$

John von Neumann (1932)

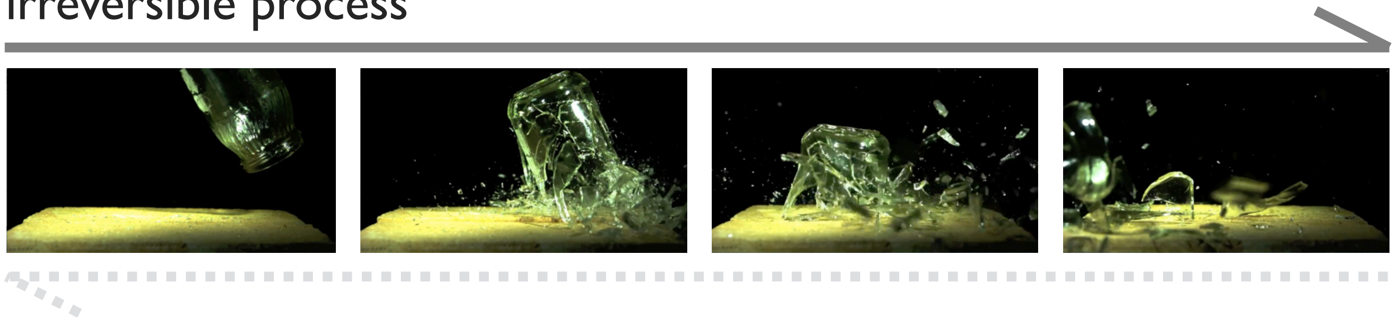
entanglement entropy…

Entropy Production

1. Irreversibility

Seifert, PRL 95, 040602 (2005)

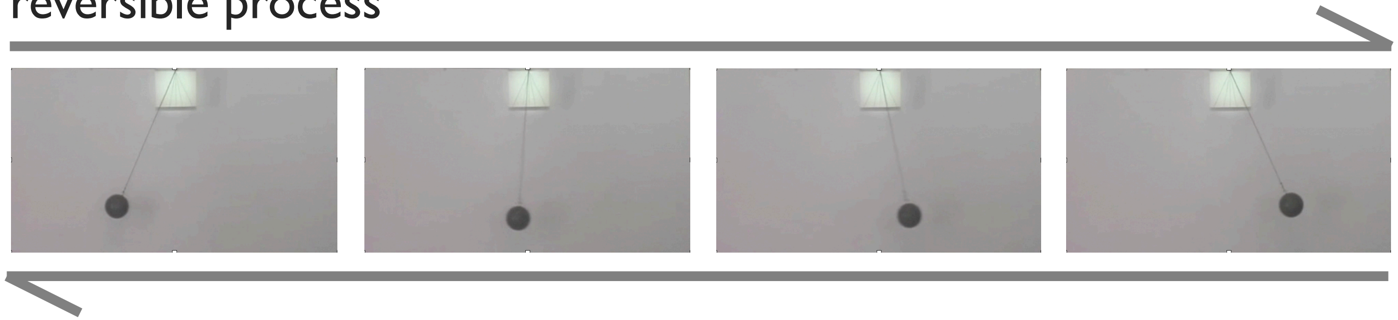
irreversible process



forward: more probable

time-reversal: less probable

reversible process



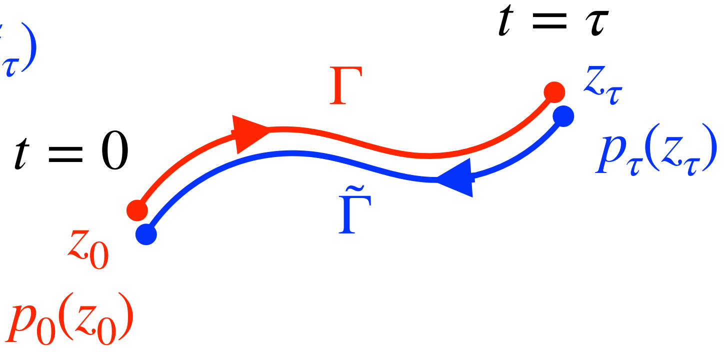
forward, time-reversal

: equally probable

Irreversibility

time-forward path probability: $\mathscr{P}(\Gamma) = p_0(z_0)\mathscr{P}(\Gamma \,|\, z_0)$

time-reverse path probability: $\tilde{\mathscr{P}}(\tilde{\Gamma}) = p_\tau(z_\tau)\tilde{\mathscr{P}}(\tilde{\Gamma} \,|\, \tilde{z}_\tau)$



$$R \equiv \ln \frac{\mathscr{P}(\Gamma)}{\tilde{\mathscr{P}}(\tilde{\Gamma})} \quad \begin{matrix} = 0 \text{ (reversible)} \\ \neq 0 \text{ (irreversible)} \end{matrix}$$

$$= \underbrace{-\ln p_\tau(z_\tau) + \ln p_0(z_0)}_{= \Delta S_{\text{sys}}} + \underbrace{\ln \frac{\mathscr{P}(\Gamma \,|\, z_0)}{\tilde{\mathscr{P}}(\tilde{\Gamma} \,|\, \tilde{z}_\tau)}}_{} = -\frac{Q}{T} = \Delta S_{\text{bath}} \quad \text{(in } k_B = 1 \text{ unit)}$$

$$= \Delta S_{\text{sys}} + \Delta S_{\text{bath}} = \Delta S_{\text{tot}} \quad \rightarrow R = \Delta S_{\text{tot}}$$: (stochastic) total entropy production!

Property of R

$$\langle e^{-R} \rangle = \sum_{\text{all paths}} \mathscr{P}(\Gamma) e^{-R} = \sum_{\text{all paths}} \tilde{\mathscr{P}}(\tilde{\Gamma}) = 1$$

➡ $\langle e^{-R} \rangle = 1$: Fluctuation Theorem

Jensen's inequality: $\langle f(x) \rangle \geq f(\langle x \rangle)$ for convex function $f(x)$

➡ $1 = \langle e^{-R} \rangle \geq e^{-\langle R \rangle} \quad \rightarrow \langle R \rangle \geq 0 \quad \rightarrow \langle \Delta S_{\text{tot}} \rangle \geq 0$

ΔS_{tot} can be negative, but its mean is nonnegative. (2nd law in stochastic systems)

Fluctuation Theorems

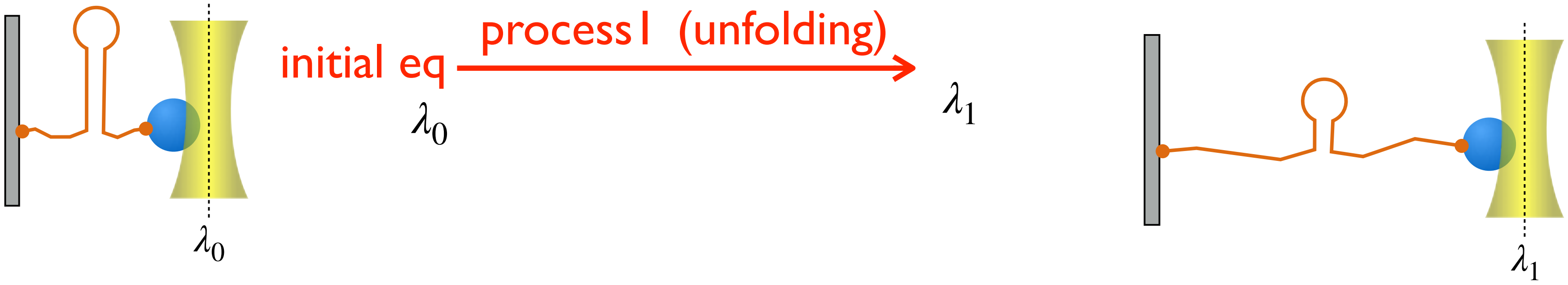
➡ $\langle e^{-R} \rangle = 1$: Fluctuation Theorem

1) $\langle e^{-\Delta S_{\mathrm{tot}}} \rangle = 1$

2) Jarzynski equality $\langle e^{-\beta W} \rangle = e^{\beta \Delta F}$

3) Hatano-Sasa FT $\Delta S_{\mathrm{tot}} = \Delta S_{\mathrm{ex}} + \Delta S_{\mathrm{hk}} \rightarrow \langle e^{-\Delta S_{\mathrm{ex}}} \rangle = 1 \quad \langle e^{-\Delta S_{\mathrm{hk}}} \rangle = 1$

4) Information FT: $\langle e^{-\Delta S_{\mathrm{tot}} + I} \rangle = 1 \rightarrow \langle \Delta S_{\mathrm{tot}} \rangle \geq \langle I \rangle$ Sagawa and Ueda, PRL 109, 180602 (2012)



initial eq $\xrightarrow{\text{process1 (unfolding)}}$

λ_0 λ_1

Expression of Entropy Production Rate

1. Overdamped Langevin system

$$\dot{x} = \frac{1}{\gamma} f(x(t), t) + \frac{1}{\gamma}\xi(t) \quad \Rightarrow \quad \partial_t P(x,t) = -\partial_x J(x,t) \qquad J(x,t) = \frac{1}{\gamma}\left(f(x,t) - k_{\mathrm{B}} T \partial_x\right) P(x,t)$$

Risken (The Fokker-Planck Equation)

$$\dot{S}_{\mathrm{sys}} = -\frac{d}{dt} k_{\mathrm{B}} \ln P(x,t) = -\frac{k_{\mathrm{B}}}{P}\frac{dP}{dt} = -\frac{k_{\mathrm{B}}}{P}\left(\underline{\partial_x P} \circ \dot{x} + \partial_t P\right)$$

$$\partial_x P = \frac{f}{k_{\mathrm{B}} T} P - \frac{\gamma}{k_{\mathrm{B}} T} J$$

$$= -\frac{f}{T} \circ \dot{x} + \frac{\gamma}{T}\frac{J}{P} \circ \dot{x} - \frac{k_{\mathrm{B}}}{P}\partial_t P$$

$$= \frac{1}{T}\underbrace{(-\gamma\dot{x} + \xi) \circ \dot{x}}_{= \dot{Q}} + \frac{\gamma}{T}\frac{J}{P} \circ \dot{x} - \frac{k_{\mathrm{B}}}{P}\partial_t P$$

$$\rightarrow \dot{S}_{\mathrm{tot}} = \dot{S}_{\mathrm{sys}} - \frac{\dot{Q}}{T} = \frac{\gamma}{T}\frac{J}{P} \circ \dot{x} - \frac{k_{\mathrm{B}}}{P}\partial_t P$$

$$\langle \cdots \rangle = \int dx \ \cdots \ P(x,t)$$

$$\rightarrow \langle \dot{S}_{\mathrm{tot}} \rangle = \frac{\gamma}{T}\left\langle \frac{J}{P} \circ \dot{x} \right\rangle - \left\langle \frac{k_{\mathrm{B}}}{P}\partial_t P \right\rangle$$

$$\left\langle \frac{k_{\mathrm{B}}}{P}\partial_t P \right\rangle = k_{\mathrm{B}} \partial_t \underbrace{\int dx P(x,t)}_{= 1} = 0$$

$$= \int dx \frac{\gamma}{T}\frac{J(x,t)^2}{P(x,t)}$$

$$\langle g(x(t), t) \circ \dot{x} \rangle = \int dx g(x,t) J(x,t)$$

Summary I

1. Irreversibility

$$R \equiv \ln \frac{\mathscr{P}(\Gamma)}{\tilde{\mathscr{P}}(\tilde{\Gamma})} \quad \begin{array}{l} = 0 \text{ (reversible)} \\ \neq 0 \text{ (irreversible)} \end{array}$$

$$= \Delta S_{\text{sys}} + \Delta S_{\text{bath}} = \Delta S_{\text{tot}}$$

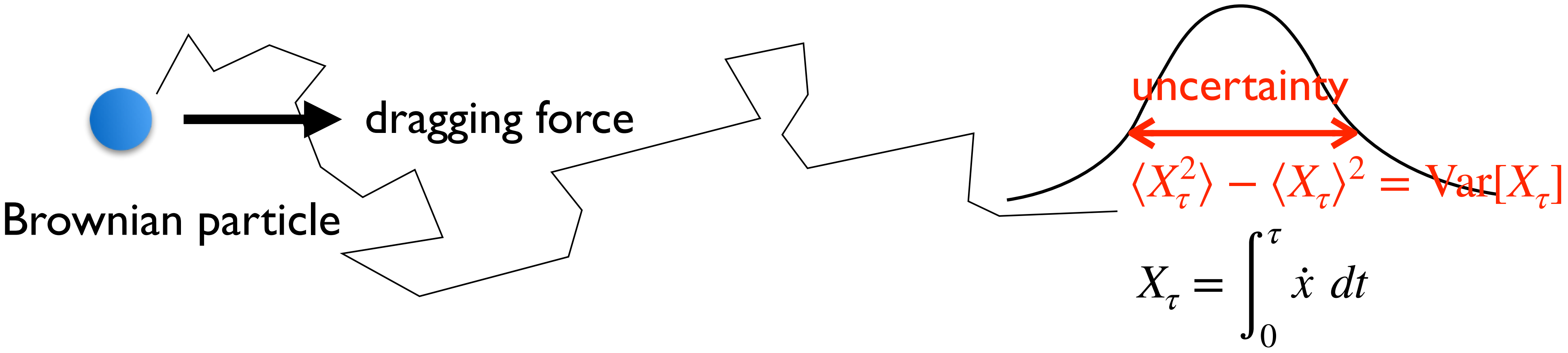
2. Fluctuation theorem: $\langle e^{-R} \rangle = 1$

3. Entropy production rate: $\langle \dot{S}_{\text{tot}} \rangle = \int dx \frac{\gamma}{T} \frac{J(x,t)^2}{P(x,t)}$

(overdamped Langevin dynamics)

Beyond the Thermodynamic Second Law

: **T**hermodynamic **U**ncertainty **R**elations (TUR)



dragging force

Brownian particle

uncertainty

$$\langle X_\tau^2\rangle - \langle X_\tau\rangle^2 = \mathrm{Var}[X_\tau]$$

$$X_\tau = \int_0^\tau \dot{x}\, dt$$

$$\underbrace{\frac{\mathrm{Var}[X_\tau]}{\langle X_\tau\rangle^2}}_{\text{relative uncertainty}}\underbrace{\langle \Delta S_{\mathrm{tot}}\rangle}_{\text{cost}} \geq 2k_{\mathrm{B}}$$

(steady state)

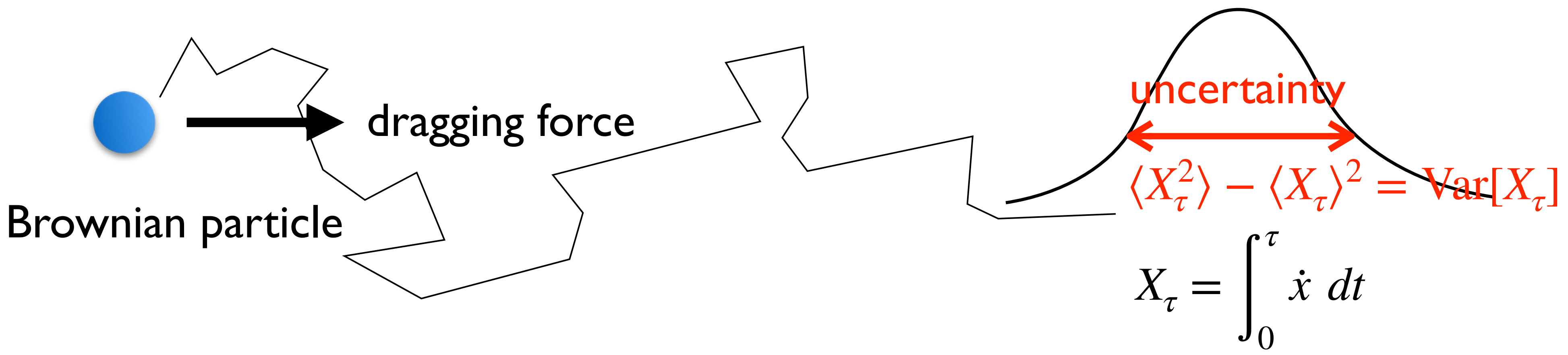
$$\frac{\mathrm{Var}[X_\tau]}{\langle X_\tau\rangle^2}\downarrow \quad \langle \Delta S_{\mathrm{tot}}\rangle \uparrow \qquad\qquad \frac{\mathrm{Var}[X_\tau]}{\langle X_\tau\rangle^2}\uparrow \quad \langle \Delta S_{\mathrm{tot}}\rangle \downarrow$$

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

Is it possible to make the uncertainty arbitrarily small?

Beyond the Thermodynamic Second Law

: **T**hermodynamic **U**ncertainty **R**elations (TUR)



dragging force

Brownian particle

uncertainty

$\langle X_\tau^2 \rangle - \langle X_\tau \rangle^2 = \mathrm{Var}[X_\tau]$

$X_\tau = \int_0^\tau \dot{x}\, dt$

For general current Θ_τ,

heat, work, displacement etc.

$$\frac{\mathrm{Var}[\Theta_\tau]}{\langle \Theta_\tau \rangle^2} \langle \Delta S_{\mathrm{tot}} \rangle \geq 2k_{\mathrm{B}}$$

(steady state)

trade-off relation btw thermodynamic cost and uncertainty of current

thermodynamic second law: $\langle \Delta S_{\mathrm{tot}} \rangle \geq 0$

TUR: stronger bound $\langle \Delta S_{\mathrm{tot}} \rangle \geq 2k_{\mathrm{B}} \dfrac{\langle \Theta_\tau \rangle^2}{\mathrm{Var}[\Theta_\tau]} > 0$

TUR - Brief History

Derivation history of TUR (2015~2019)

- first report in 2015 Barato et al, PRL 114, 158101 (2015)
- first proof via large deviation theory in 2016 Gingrich et al, PRL 116, 120601 (2016)
  Horowitz and Gingrich, PRE 96, 020103(R) (2017)
- proof via generating function method in 2018 Dechant and Sasa, J Stat Mech 063209 (2018)
- proof via Cramér-Rao inequality in 2019 Hasegawa and Vu, PRE 99, 062126 (2019)

$$\frac{\mathrm{Var}_\epsilon[\Theta]}{\left(\partial_\epsilon \langle \Theta \rangle_\epsilon\right)^2} \geq \frac{1}{\mathcal{I}(\epsilon)}$$

$\mathcal{I}(\epsilon)$: Fisher information

This greatly simplifies the TUR derivation.

Cramér-Rao Inequality

$\Theta(z)$: observable

$P_\epsilon(z)$: probability distribution → $\langle\cdots\rangle_\epsilon = \int dz\ \cdots\ P_\epsilon(z)$ → $\langle\Theta\rangle_\epsilon = \int dz\ \Theta(z)P_\epsilon(z)$

$$\left(\partial_\epsilon\langle\Theta\rangle_\epsilon\right)^2 = \left(\int dz\ \Theta(z)\partial_\epsilon P_\epsilon(z)\right)^2$$

note : $\int dz\ \langle\Theta\rangle_\epsilon\partial_\epsilon P_\epsilon(z) = \langle\Theta\rangle_\epsilon\partial_\epsilon\int dz\ P_\epsilon(z) = 0$

$$= \left(\int dz\ \Theta(z)\partial_\epsilon P_\epsilon(z) - \int dz\ \langle\Theta\rangle_\epsilon\partial_\epsilon P_\epsilon(z)\right)^2$$

$$= \left(\int dz\ \left[\Theta(z) - \langle\Theta\rangle_\epsilon\right]\ \underline{\partial_\epsilon P_\epsilon(z)}\right)^2$$

$\partial_\epsilon P_\epsilon(z) = P_\epsilon(z)\partial_\epsilon \ln P_\epsilon(z)$

$$= \left(\int dz\ \left[\Theta(z) - \langle\Theta\rangle_\epsilon\right]\left[\partial_\epsilon \ln P_\epsilon(z)\right]\ P_\epsilon(z)\right)^2$$

Cauchy-Schwarz $(\mathbf{a}\cdot\mathbf{c})^2 \leq |\mathbf{a}|^2|\mathbf{c}|^2$

$$\leq \underbrace{\int dz\left[\Theta(z) - \langle\Theta\rangle_\epsilon\right]^2 P_\epsilon(z)}_{= \mathrm{Var}_\epsilon[\Theta]}\ \underline{\int dz\left[\partial_\epsilon \ln P_\epsilon(z)\right]^2 P_\epsilon(z)}$$

$$= \int dz\ \partial_\epsilon \ln P_\epsilon(z)\ \partial_\epsilon \ln P_\epsilon(z)\ P_\epsilon(z)$$

$$= \int dz\ \partial_\epsilon \ln P_\epsilon(z)\ \partial_\epsilon P_\epsilon(z) = -\int dz\ \partial_\epsilon^2 \ln P_\epsilon(z)\ P_\epsilon(z)$$

$$= -\langle\partial_\epsilon^2 \ln P_\epsilon(z)\rangle_\epsilon \equiv \mathcal{I}(\epsilon)$$

$$= \mathrm{Var}_\epsilon[\Theta]\mathcal{I}(\epsilon)$$

➡ $$\frac{\mathrm{Var}_\epsilon[\Theta]}{\left(\partial_\epsilon\langle\Theta\rangle_\epsilon\right)^2} \geq \frac{1}{\mathcal{I}(\epsilon)}$$

Cramér-Rao Inequality

$\Theta(z)$: observable $\quad\rightarrow\quad \Theta(\Gamma)$: observable (work, heat, displacement, etc.)

$P_\epsilon(z)$: probability distribution $\quad\rightarrow\quad \mathscr{P}_\epsilon(\Gamma)$: path probability

$$\frac{\mathrm{Var}_\epsilon[\Theta]}{\left(\partial_\epsilon\langle\Theta\rangle_\epsilon\right)^2} \geq \frac{1}{\mathscr{I}(\epsilon)} \longrightarrow \frac{\mathrm{Var}_\epsilon[\Theta]\,|_{\epsilon=0}}{\left(\partial_\epsilon\langle\Theta\rangle_\epsilon\,|_{\epsilon=0}\right)^2} \geq \frac{1}{\mathscr{I}(0)} \Longleftrightarrow \frac{\mathrm{Var}[\Theta]}{\langle\Theta\rangle^2}\langle S_{\mathrm{tot}}\rangle \geq 2k_{\mathrm{B}}$$

$$\rightarrow \mathrm{Var}_\epsilon[\Theta]\,|_{\epsilon=0} = \mathrm{Var}[\Theta]$$

$$\boxed{\begin{aligned} &\rightarrow \partial_\epsilon\langle\Theta\rangle_\epsilon\,|_{\epsilon=0} = \langle\Theta\rangle \\ &\rightarrow \mathscr{I}(0) = \frac{\langle S_{\mathrm{tot}}\rangle}{2k_{\mathrm{B}}} \end{aligned}}$$

original dynamics: $\gamma\dot{x} = F(x) + \xi$

ε-perturbed dynamics: (e.g.) $\gamma\dot{x} = F(x) + \epsilon G(x) + \xi$ $\quad(\epsilon \rightarrow 0$: original)

TUR Derivation for Overdamped Langevin Dynamics

What perturbation leads to these?

$$\boxed{\begin{aligned}&\to \partial_\epsilon \langle \Theta \rangle_\epsilon |_{\epsilon=0} = \langle \Theta \rangle \\ &\to \mathcal{I}(0) = \frac{\langle S_{\mathrm{tot}} \rangle}{2k_{\mathrm{B}}}\end{aligned}}$$

$$\Rightarrow \langle \Theta \rangle_\epsilon = (1+\epsilon)\langle \Theta \rangle$$

In a steady state:

$$\langle \Theta \rangle^{\mathrm{ss}} = \tau \langle \dot{\Theta} \rangle^{\mathrm{ss}} \quad (0 \le t \le \tau) \qquad \tau \to (1+\epsilon)\tau : \langle \Theta \rangle^{\mathrm{ss}}_\epsilon = (1+\epsilon)\tau \langle \dot{\Theta} \rangle^{\mathrm{ss}}$$

∴ time scaling perturbation : $t \to (1+\epsilon)t$

Equivalent to time perturbation

original dynamics: $\gamma \dot{x} = F(x) + \xi$

$$\boxed{\to \text{perturbed dynamics:} \quad \gamma \dot{x} = F(x) + \epsilon G(x) + \xi}$$

Fokker-Planck equation: $\partial_t P(x,t) = -\partial_x \gamma^{-1}(F(x) - k_{\mathrm{B}} T \partial_x) P(x,t)$

perturbed FP equation: $\partial_t P(x,(1+\epsilon)t) = -(1+\epsilon)\partial_x \gamma^{-1}(F(x) - k_{\mathrm{B}} T \partial_x) P(x,(1+\epsilon)t)$

steady state: $\partial_t P^{\mathrm{ss}}(x) = 0 = -(1+\epsilon)\partial_x \underline{\gamma^{-1}(F(x) - k_{\mathrm{B}} T \partial_x) P^{\mathrm{ss}}(x)}$

$$J^{\mathrm{ss}}(x) = \gamma^{-1}\left(F(x) - k_{\mathrm{B}} T \partial_x\right) P^{\mathrm{ss}}(x)$$

$$= -\partial_x \gamma^{-1}(F(x) - k_{\mathrm{B}} T \partial_x) P^{\mathrm{ss}}(x) - \partial_x \epsilon J^{\mathrm{ss}}(x)$$

$$= -\partial_x \gamma^{-1}\left(F(x) + \epsilon \frac{\gamma J^{\mathrm{ss}}(x)}{\underline{P^{\mathrm{ss}}(x)}} - k_{\mathrm{B}} T \partial_x\right) P^{\mathrm{ss}}(x) \qquad G(x) \equiv \frac{\gamma J^{\mathrm{ss}}(x)}{P^{\mathrm{ss}}(x)}$$

TUR Derivation for Overdamped Langevin Dynamics

What perturbation leads to these?

$$\Rightarrow \langle\Theta\rangle_\epsilon = (1+\epsilon)\langle\Theta\rangle$$

$$\boxed{\begin{aligned}&\to \partial_\epsilon\langle\Theta\rangle_\epsilon\big|_{\epsilon=0} = \langle\Theta\rangle\\ &\to \mathcal{I}(0) = \frac{\langle S_{\mathrm{tot}}\rangle}{2k_{\mathrm{B}}}\end{aligned}}$$

→ these are satisfied.

In a steady state:

→ perturbed dynamics: $\gamma\dot{x} = F(x)+\epsilon G(x)+\xi$ $\qquad G(x) \equiv \frac{\gamma J^{\mathrm{ss}}(x)}{P^{\mathrm{ss}}(x)}$

Fisher information

$$\mathcal{I}(\epsilon) = -\langle\partial_\epsilon^2 \ln \mathcal{P}_\epsilon(\Gamma)\rangle_\epsilon = \left\langle \partial_\epsilon^2\int_0^\tau dt\,\frac{\gamma}{4k_{\mathrm{B}}T}\left(\dot{x} - \frac{F(x)+\epsilon G(x)}{\gamma}\right)^2\right\rangle_\epsilon$$

$$\boxed{\mathcal{P}_\epsilon(\Gamma) = \prod_{n=0}^{N}\left(\frac{dx(t_n)}{\sqrt{4\pi k_{\mathrm{B}}T/\gamma}}\right)\exp\left[\int_0^\tau dt\left(-\frac{1}{4k_{\mathrm{B}}T/\gamma}\left\{\dot{x} - F(x)/\gamma - \epsilon G(x)/\gamma\right\}_{\bullet}^{2}\right)\right]p_0(x(0))}$$

$a = 1$ (Ito)

$$= \left\langle \partial_\epsilon^2\int_0^\tau dt\,\frac{\gamma}{4k_{\mathrm{B}}T}\left[\left(\dot{x} - \frac{F(x)}{\gamma}\right)^2 + 2\left(\dot{x} - \frac{F(x)}{\gamma}\right)\frac{\epsilon G(x)}{\gamma} + \left(\frac{\epsilon G(x)}{\gamma}\right)^2\right]\right\rangle_\epsilon$$

$$= \int_0^\tau dt\left\langle\frac{G^2(x)}{2\gamma k_{\mathrm{B}}T}\right\rangle_\epsilon = \frac{1}{2k_{\mathrm{B}}}\int_0^\tau dt\,\underset{=\langle\dot{S}_{\mathrm{tot}}\rangle}{\boxed{\int dx\,\frac{\gamma}{T}\frac{J^{\mathrm{ss}}(x)^2}{P^{\mathrm{ss}}(x)}}} = \frac{\langle S_{\mathrm{tot}}\rangle^{\mathrm{ss}}}{2k_{\mathrm{B}}}$$

$$\langle\cdots\rangle_\epsilon = \int_x \cdots\, P_\epsilon(x)^{\mathrm{ss}} \qquad (P_\epsilon(x)^{\mathrm{ss}} = P^{\mathrm{ss}}(x))$$

TUR Derivation for Overdamped Langevin Dynamics

$$\frac{\mathrm{Var}_\epsilon[\Theta]\,|_{\epsilon=0}}{\left(\partial_\epsilon \langle\Theta\rangle_\epsilon\,|_{\epsilon=0}\right)^2} \geq \frac{1}{\mathcal{I}(0)} \quad \Longleftrightarrow \quad \frac{\mathrm{Var}[\Theta]}{\langle\Theta\rangle^2}\langle S_{\mathrm{tot}}\rangle \geq 2k_{\mathrm{B}}$$

$$\to \mathrm{Var}_\epsilon[\Theta]\,|_{\epsilon=0} = \mathrm{Var}[\Theta]$$

$$\boxed{\begin{aligned} &\to \partial_\epsilon \langle\Theta\rangle_\epsilon\,|_{\epsilon=0} = \langle\Theta\rangle \\ &\to \mathcal{I}(0) = \frac{\langle S_{\mathrm{tot}}\rangle}{2k_{\mathrm{B}}} \end{aligned}}$$

TUR and Variants of TUR

Steady-state TUR (overdamped Langevin system + Markov jump process)

$$\frac{\mathrm{Var}[\Theta_\tau]}{\langle \Theta_\tau \rangle^2} \langle \Delta S_{\mathrm{tot}} \rangle \geq 2k_{\mathrm{B}}$$ (steady state)

Dechant and Sasa, JStatMech 063209 (2018)
Hasegawa and Vu, PRE 99, 062126 (2019)

TUR with an arbitrary state (overdamped Langevin system + Markov jump process)

$$\frac{\mathrm{Var}[\Theta_\tau]}{(\hat{h}_{\mathrm{o}} \langle \Theta_\tau \rangle)^2} \langle \Delta S_{\mathrm{tot}} \rangle \geq 2k_{\mathrm{B}}$$ (arbitrary time-dependent protocol)

Koyuk and Seifert, PRL 125, 260604 (2020)

$$\hat{h}_{\mathrm{o}} \equiv \tau \partial_\tau - \omega \partial_\omega \quad (\tau: \ \text{final time}, \ \ \omega: \ \text{protocol change speed})$$

TUR with an arbitrary state (underdamped Langevin system)

$$\frac{\mathrm{Var}[\Theta_\tau]}{(\hat{h}_{\mathrm{u}} \langle \Theta_\tau \rangle)^2} \langle \Delta S_{\mathrm{tot}} \rangle \geq 2k_{\mathrm{B}}$$ (arbitrary time-dependent protocol)

JSL, Park, Park, PRE 104, L052102 (2021)
Kwon, Park, JSL, Baek, arXiv:2311.01098

$$\hat{h}_{\mathrm{u}} = \tau \partial_\tau - s \partial_s - \omega \partial_\omega$$

Summary2

1. TUR (for overdamped systems in steady-state)

$$\frac{\mathrm{Var}[\Theta_\tau]}{\langle \Theta_\tau \rangle^2} \langle \Delta S_{\mathrm{tot}} \rangle \geq 2k_{\mathrm{B}}$$

: trade-off relation btw thermodynamic cost and uncertainty of current

Application of TUR

Estimation of entropy production: How to measure?

1. using definition of entropy production

$$\Delta S_{\mathrm{tot}} \equiv \ln \frac{\mathscr{P}(\Gamma)}{\tilde{\mathscr{P}}(\tilde{\Gamma})}$$

: not possible to measure all trajectories

2. using TUR

$$\langle \Delta S_{\mathrm{tot}} \rangle \geq 2k_{\mathrm{B}} \frac{\langle \Theta_\tau \rangle^2}{\mathrm{Var}[\Theta_\tau]} \equiv B[\Theta_\tau]$$

- pros: experimentally feasible (measurable current)
- cons: not exact, but bound
- study to find Θ_{max} which makes *B* maximum: tightest

Application of TUR

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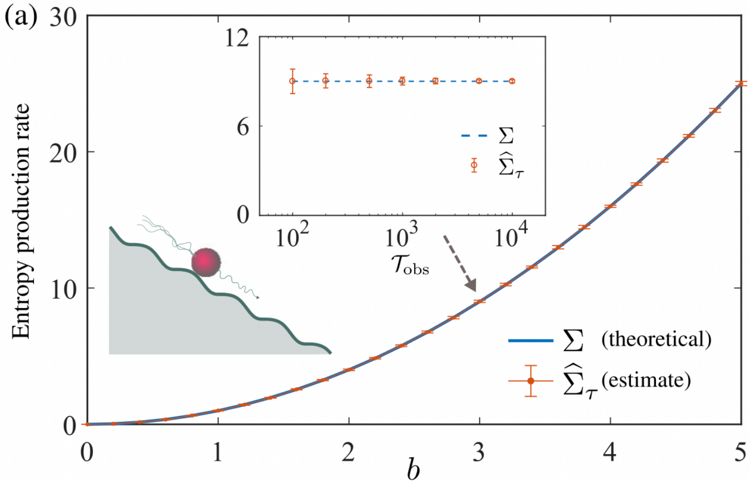


periodically driven particle

Vu, Vo, Hasegawa, PRE 101, 042138 (2020)

3. multidimensional entropic bound Lee, JSL et al., PRR 5, 013194 (2023)

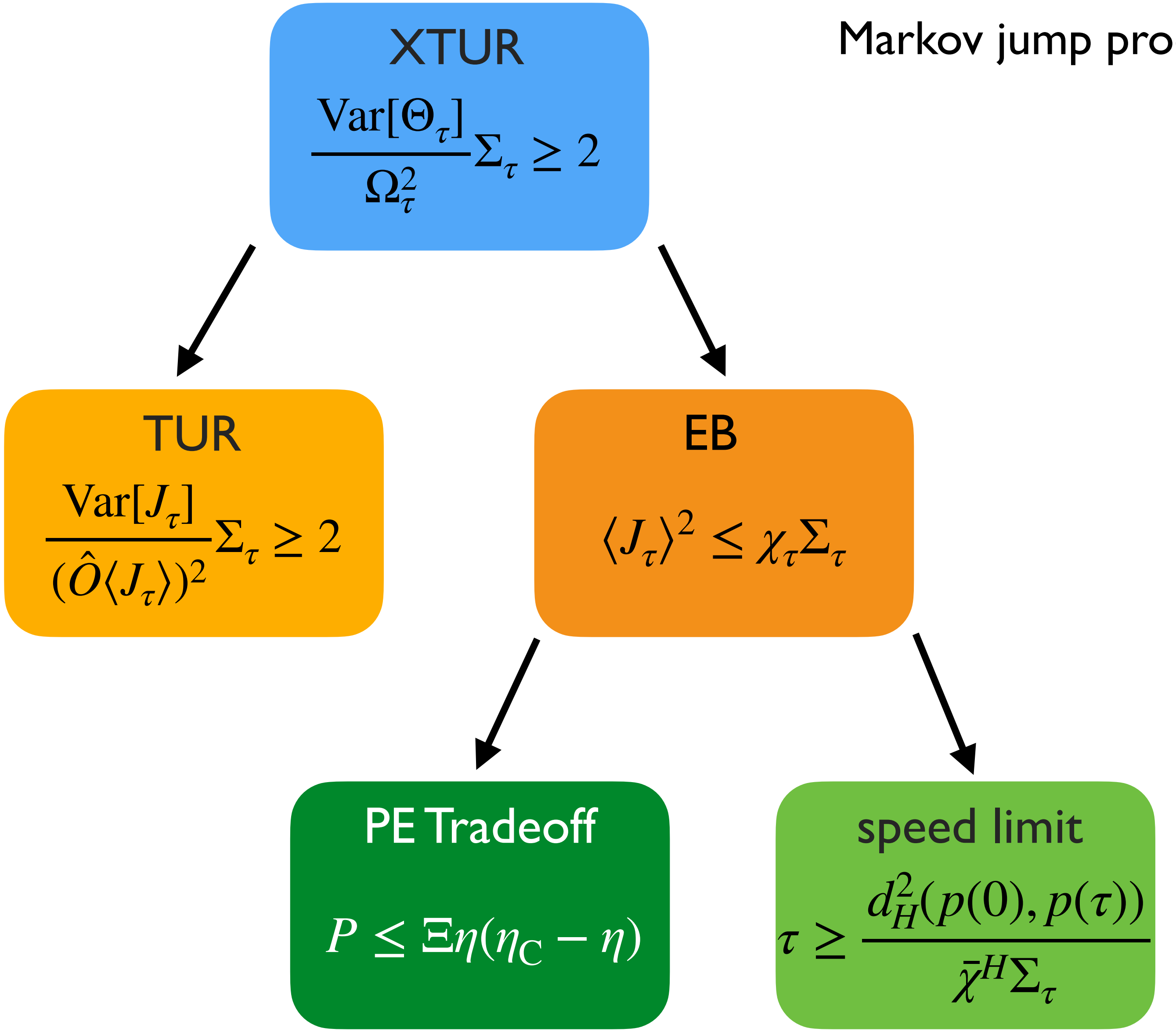
4. Using machine learning technique Kim et al., PRL 125, 140605 (2020)

Unified Hierarchical Relationship

Kwon, Park, JSL, Baek, PRE 110, 044131 (2024)

valid for Langevin systems

Markov jump processes



XTUR

$$\frac{\mathrm{Var}[\Theta_\tau]}{\Omega_\tau^2}\Sigma_\tau \geq 2$$

TUR

$$\frac{\mathrm{Var}[J_\tau]}{(\hat{O}\langle J_\tau\rangle)^2}\Sigma_\tau \geq 2$$

EB

$$\langle J_\tau\rangle^2 \leq \chi_\tau\Sigma_\tau$$

PE Tradeoff

$$P \leq \Xi\eta(\eta_{\mathrm{C}} - \eta)$$

speed limit

$$\tau \geq \frac{d_H^2(p(0), p(\tau))}{\bar{\chi}^H\Sigma_\tau}$$

Extension to Quantum Systems

Quantum Jarzynski equality

Campisi et al, Rev Mod Phys 83, 771 (2011)

$\langle e^{-\beta W} \rangle = e^{\beta \Delta F}$ for isolated quantum system (unitary evolution)

Quantum Fluctuation Theorem with Information

Yada, Yoshioka, Sagawa, PRL 128, 170601 (2022)

$$\langle e^{-\beta(\Delta S_{\mathrm{tot}} + I_{\mathrm{QC}})} \rangle = 1 \quad \rightarrow \langle \Delta S_{\mathrm{tot}} \rangle \geq -\langle I_{\mathrm{QC}} \rangle$$

Quantum TUR

Vu, Saito, PRL 128, 140602 (2022)

$$\frac{\mathrm{Var}[\Theta_\tau]}{\langle \Theta_\tau \rangle} \geq \frac{2(1+\delta J)^2}{\Delta S_{\mathrm{tot}} + 2Q_1} \quad \rightarrow \frac{\mathrm{Var}[\Theta_\tau]}{\langle \Theta_\tau \rangle} \geq \frac{2(1+\delta)^2}{\Delta S_{\mathrm{tot}}}$$

in preparation

Quantum Speed Limit

Vu, Saito, PRX 13, 011013 (2023)

$$\tau \geq \frac{\mathscr{W}_q(\rho(0), \rho(\tau))}{\sqrt{\langle m \rangle_\tau \langle \dot{S}_{\mathrm{tot}} \rangle_\tau}}$$

Quantum fluctuation-response inequality

Kwon, Chun, Par, JSL, arXiv:2411.18108

$$\sum_{k=1}^{K} \frac{R_{\theta_k}^2(\tau)}{\tau a_k} \leq \mathrm{Var}(\Theta_\tau)$$