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

Lecture 3

2022 ICTP-KIAS School on Statistical Physics for Life Sciences

October 31- November 7, 2022

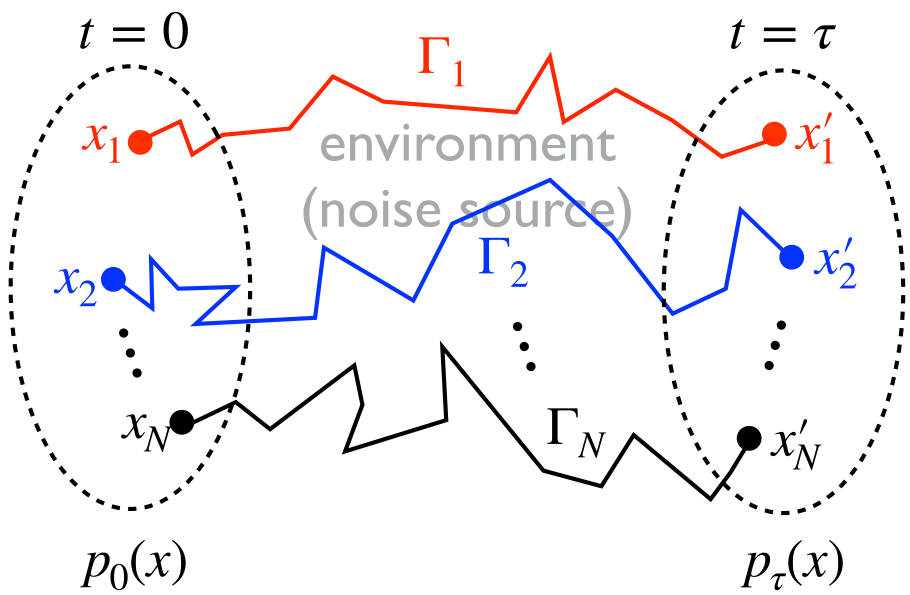
Jae Sung Lee

Korea Institute for Advanced Study

Q

Is there any general relation
for EP and measurable observables?

Schematic of a stochastic system



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

Lecture 1

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

Lecture 2

I. Fluctuation Theorems Lecture 2

: relation for EP

$e^{-\langle \Sigma \rangle / k_B} \leq \langle e^{-\Sigma / k_B} \rangle = 1$: generalized 2nd law

Jesen's inequality

$\to \langle \Sigma \rangle \geq 0$: thermodynamic 2nd law

Various FTs

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

Jarzynski, PRL 78, 2690 (1997)

Crooks FT $P(W)/P(-W) = e^{\beta(W - \Delta F)}$

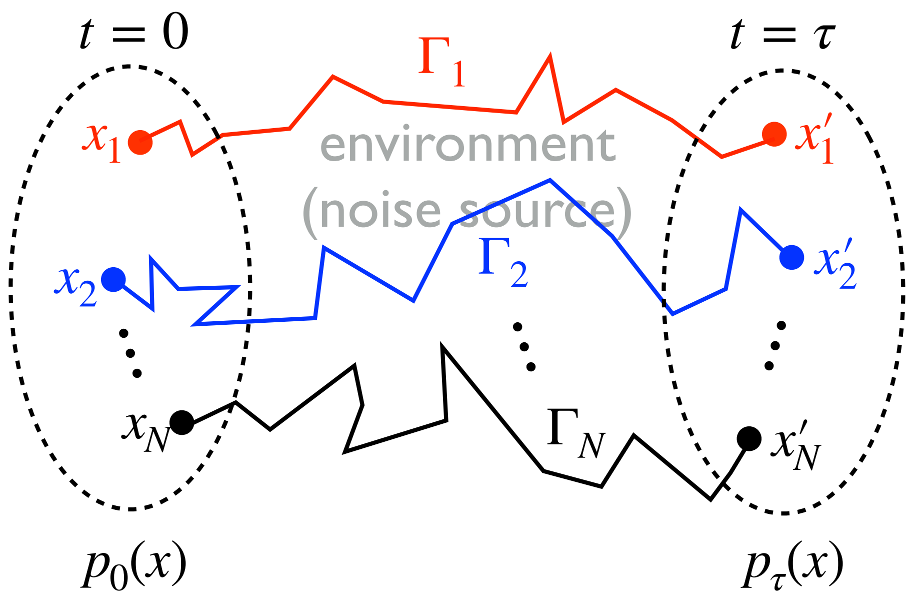
Crooks, PRE 60, 2721 (1999)

Hatano-Sasa FT $\langle e^{-\Sigma_a} \rangle = 1, \ \langle e^{-\Sigma_{na}} \rangle = 1$

Hatano and Sasa, PRL 86, 3463 (2001)

Information FT $\langle e^{-\Sigma + I} \rangle = 1$ Sagawa and Ueda, PRL 109, 180602 (2012)

Schematic of a stochastic system



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

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

2. TUR (Thermodynamic Uncertainty Relations) Lecture 3

: relation of EP and fluctuation of Θ

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

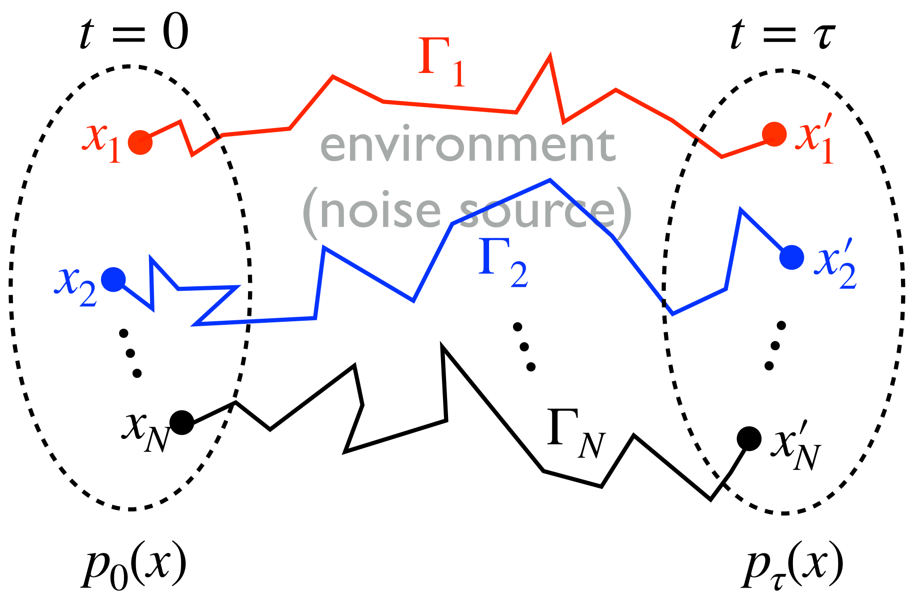
$$\boxed{\frac{\mathrm{Var}[X_\tau]}{\langle X_\tau\rangle^2}\downarrow \quad \langle\Sigma\rangle\uparrow \qquad \frac{\mathrm{Var}[X_\tau]}{\langle X_\tau\rangle^2}\uparrow \quad \langle\Sigma\rangle\downarrow}$$

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

$$\langle\Sigma\rangle \geq 2k_\mathrm{B}\frac{\langle\Theta\rangle^2}{\mathrm{Var}[\Theta]} \geq 0$$

stronger than the thermodynamic second law

Schematic of a stochastic system



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

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

Contents of Lecture 3

1. TUR derivation

   - Cramér-Rao inequality

   - TUR derivation for overdamped Langevin System

   - TUR derivation for Markovian jump process

   - Variants of TUR

2. TUR application

   - Estimation of entropy production

   - Estimation of extent of anomalous diffusion

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)

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

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

This greatly simplifies the TUR derivation.

Cramér-Rao Inequality

$\Theta(z)$: observable

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

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

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

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

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

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

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

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

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

Cramér-Rao Inequality

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

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

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

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

$$\boxed{\begin{array}{l} \rightarrow \partial_\epsilon \langle \Theta \rangle_\epsilon |_{\epsilon=0} = \langle \Theta \rangle \\ \rightarrow \mathcal{I}(0) = \dfrac{\langle \Sigma \rangle}{2k_\mathrm{B}} \end{array}}$$

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

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

TUR Derivation for Overdamped Langevin Dynamics

What perturbation leads to these?

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

$$\boxed{\begin{aligned} &\rightarrow \partial_\epsilon \langle \Theta \rangle_\epsilon |_{\epsilon=0} = \langle \Theta \rangle \\ &\rightarrow \mathcal{I}(0) = \frac{\langle \Sigma \rangle}{2k_B} \end{aligned}}$$

In a steady state:

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

$\therefore$ time scaling perturbation : $t \rightarrow (1+\epsilon)t$

Equivalent to time perturbation

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

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

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

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

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

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

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

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

TUR Derivation for Overdamped Langevin Dynamics

What perturbation leads to these?

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

$$\boxed{\begin{array}{l} \to \partial_\epsilon \langle\Theta\rangle_\epsilon |_{\epsilon=0} = \langle\Theta\rangle \\ \to \mathcal{I}(0) = \dfrac{\langle\Sigma\rangle}{2k_B} \end{array}}$$

$\to$ these are satisfied.

In a steady state:

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

Fisher information

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

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

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

$$= \int_0^\tau dt \left\langle \frac{G^2(x)}{2\gamma k_BT}\right\rangle_\epsilon = \frac{1}{2k_B}\int_0^\tau dt \underbrace{\boxed{\int dx \frac{\gamma}{T}\frac{J^{ss}(x)^2}{P^{ss}(x)}}}_{=\langle\dot{\Sigma}\rangle} = \frac{\langle\Sigma\rangle^{ss}}{2k_B}$$

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

TUR Derivation for Overdamped Langevin Dynamics

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

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

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

TUR Derivation for Markov Jump Process

What perturbation leads to these?

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

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

In a steady state:

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

$\therefore$ time scaling perturbation : $t \rightarrow (1+\epsilon)t$

original dynamics: $$\frac{d}{dt}p_x(t) = \sum_{y(\neq x)} \Big(R_{xy}p_y(t) - R_{yx}p_x(t)\Big)$$

perturbed dynamics: $$\frac{d}{dt}p_x((1+\epsilon)t) = (1+\epsilon)\sum_{y(\neq x)} \Big(R_{xy}p_y((1+\epsilon)t) - R_{yx}p_x((1+\epsilon)t)\Big)$$

steady state:

$$\frac{d}{dt}p_x^{\mathrm{ss}} = 0 = \sum_{y(\neq x)} \Big((1+\epsilon)R_{xy}p_y^{\mathrm{ss}} - (1+\epsilon)R_{yx}p_x^{\mathrm{ss}}\Big)$$

$$= \sum_{y(\neq x)} \left((1+\epsilon)R_{xy}p_y^{\mathrm{ss}} - (1+\epsilon)R_{yx}p_x^{\mathrm{ss}} - R_{xy}p_y^{\mathrm{ss}}\underbrace{\frac{2R_{yx}p_x^{\mathrm{ss}}}{R_{xy}p_y^{\mathrm{ss}} + R_{yx}p_x^{\mathrm{ss}}}}_{\equiv \eta_{xy}}\epsilon + R_{yx}p_x^{\mathrm{ss}}\underbrace{\frac{2R_{xy}p_y^{\mathrm{ss}}}{R_{xy}p_y^{\mathrm{ss}} + R_{yx}p_x^{\mathrm{ss}}}}_{= \eta_{yx}}\epsilon\right)$$

$$= \sum_{y(\neq x)} \Big[\{1+\epsilon(1-\eta_{xy})\}R_{xy}p_y^{\mathrm{ss}} - \{1+\epsilon(1-\eta_{yx})\}R_{yx}p_x^{\mathrm{ss}}\Big]$$

TUR Derivation for Markov Jump Process

What perturbation leads to these?

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

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

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 : $t \to (1+\epsilon)t$

original dynamics: $\displaystyle \frac{d}{dt} p_x(t) = \sum_{y(\neq x)} \Big(R_{xy} p_y(t) - R_{yx} p_x(t) \Big)$

perturbed dynamics: $\displaystyle \frac{d}{dt} p_x((1+\epsilon)t) = (1+\epsilon) \sum_{y(\neq x)} \Big(R_{xy} p_y((1+\epsilon)t) - R_{yx} p_x((1+\epsilon)t) \Big)$

steady state:

$$\frac{d}{dt} p_x^{\mathrm{ss}} = 0 = \sum_{y(\neq x)} \Big((1+\epsilon) R_{xy} p_y^{\mathrm{ss}} - (1+\epsilon) R_{yx} p_x^{\mathrm{ss}} \Big)$$

$$= \sum_{y(\neq x)} \Big[\{1 + \epsilon(1-\eta_{xy})\} R_{xy} p_y^{\mathrm{ss}} - \{1 + \epsilon(1-\eta_{yx})\} R_{yx} p_x^{\mathrm{ss}} \Big] \qquad \eta_{xy} \equiv \frac{2R_{yx} p_x^{\mathrm{ss}}}{R_{xy} p_y^{\mathrm{ss}} + R_{yx} p_x^{\mathrm{ss}}}$$

→ perturbed dynamics: $\displaystyle \dot{p}_x = \sum_{y(\neq x)} \Big[R^\epsilon_{xy} p_y - R^\epsilon_{yx} p_x \Big]$

$$R^\epsilon_{xy} = [1 + \epsilon(1 - \eta_{xy}\delta)] R_{xy}$$

$$\delta = 0 \text{ or } 1$$

TUR Derivation for Markov Jump Process

What perturbation leads to these?

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

$$\boxed{\begin{aligned} &\to \partial_\epsilon \langle \Theta \rangle_\epsilon |_{\epsilon=0} = \langle \Theta \rangle \\ &\to \mathcal{I}(0) = \frac{\langle \Sigma \rangle}{2k_B} \end{aligned}}$$

$\to$ these are satisfied.

In a steady state:

$\to$ perturbed dynamics: $\dot{p}_x = \sum_{y(\neq x)} \left[R^\epsilon_{xy} p_y - R^\epsilon_{yx} p_x \right]$

$$\eta_{xy} \equiv \frac{2 R_{yx} p_x^{ss}}{R_{xy} p_y^{ss} + R_{yx} p_x^{ss}}$$

$$R^\epsilon_{xy} = [1 + \epsilon(1 - \eta_{xy}\delta)] R_{xy} \quad \delta = 0 \text{ or } 1$$

Fisher information

$$\mathcal{I}(\epsilon) = -\langle \partial_\epsilon^2 \ln \mathcal{P}_\epsilon(\Gamma) \rangle_\epsilon$$

$$\mathcal{P}_\epsilon(\Gamma) = p_{x_0}(0) \prod_{n=1}^{N} \left[\underline{e^{\int_{t_{n-1}}^{t_n} R^\epsilon_{x_{n-1},x_{n-1}} dt}} \, \underline{R^\epsilon_{x_{n-1},x_n}(t_n) dt} \right] \underline{e^{\int_{t_N}^{\tau} R^\epsilon_{x_N,x_N} dt}}$$

$$\exp\left[\int_0^\tau dt \sum_x R^\epsilon_{xx} \delta_{x(t),x} \right] \qquad \exp\left[\int_0^\tau dt \sum_{x \neq y} \dot{m}_{xy}(t) \ln R^\epsilon_{xy} \right] \qquad \dot{m}_{xy}(t) = \sum_n \delta(t - t_{xy}^{(n)})$$

$t_{xy}^{(n)}$: time at which transition $y \to x$ occurs

$$\mathcal{P}_\epsilon(\Gamma) = p_{x_0}(0) \exp\left[\int_0^\tau dt \sum_x R^\epsilon_{xx} \delta_{x(t),x} + \int_0^\tau dt \sum_{x \neq y} \dot{m}_{xy}(t) \ln R^\epsilon_{xy} \right]$$

$$\langle \delta_{x(t),x} \rangle_\epsilon = p_x^\epsilon(t)$$

$$\langle \dot{m}_{xy}(t) \rangle_\epsilon = R^\epsilon_{xy} p_y^\epsilon(t)$$

TUR Derivation for Markov Jump Process

What perturbation leads to these?

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

$$\boxed{\begin{aligned}&\to \partial_\epsilon\langle\Theta\rangle_\epsilon|_{\epsilon=0} = \langle\Theta\rangle\\ &\to \mathcal{I}(0) = \frac{\langle\Sigma\rangle}{2k_B}\end{aligned}}$$

$\to$ these are satisfied.

In a steady state:

$\to$ perturbed dynamics: $\dot{p}_x = \sum_{y(\neq x)}\left[R^\epsilon_{xy}p_y - R^\epsilon_{yx}p_x\right]$

$$\eta_{xy} \equiv \frac{2R_{yx}p^{ss}_x}{R_{xy}p^{ss}_y + R_{yx}p^{ss}_x}$$

$$R^\epsilon_{xy} = [1+\epsilon(1-\eta_{xy}\delta)]R_{xy} \qquad \delta = 0 \text{ or } 1$$

Fisher information

$$\mathcal{I}(\epsilon) = -\langle\partial^2_\epsilon \ln\mathcal{P}_\epsilon(\Gamma)\rangle_\epsilon \;= -\left\langle \int_0^\tau dt\sum_x \cancel{\partial^2_\epsilon R^\epsilon_{xx}}\delta_{x(t),x} + \int_0^\tau dt\sum_{x,y}\dot{m}_{xy}(t)\partial^2_\epsilon \ln R^\epsilon_{xy}\right\rangle_\epsilon$$

$$\boxed{\mathcal{P}_\epsilon(\Gamma) = p_{x_0}(0)\exp\left[\int_0^\tau dt\sum_x R^\epsilon_{xx}\delta_{x(t),x} + \int_0^\tau dt\sum_{x\neq y}\dot{m}_{xy}(t)\ln R^\epsilon_{xy}\right] \qquad \begin{aligned}\langle\delta_{x(t),x}\rangle_\epsilon &= p^\epsilon_x(t)\\ \langle\dot{m}_{xy}(t)\rangle_\epsilon &= R^\epsilon_{xy}p^\epsilon_y(t)\end{aligned}}$$

$$= -\int_0^\tau dt\sum_{x\neq y}\langle\dot{m}_{xy}(t)\rangle_\epsilon \frac{(\cancel{\partial^2_\epsilon R^\epsilon_{xy}})R^\epsilon_{xy} - (\partial_\epsilon R^\epsilon_{xy})^2}{(R^\epsilon_{xy})^2}$$

$= \dot{A}(t)$: dynamical activity

$$\mathcal{I}(0) = \int_0^\tau dt\sum_{x\neq y}R_{xy}p^{ss}_y\frac{(1-\eta_{xy}\delta)^2(R_{xy})^2}{(R_{xy})^2} = \int_0^\tau dt\,\boxed{\sum_{x\neq y}R_{xy}p^{ss}_y} = A(\tau) \qquad (\delta = 0)$$

$$= \int_0^\tau dt\sum_{x\neq y}R_{xy}p^{ss}_y\left(\frac{R_{xy}p^{ss}_y - R_{yx}p^{ss}_x}{R_{xy}p^{ss}_y + R_{yx}p^{ss}_x}\right)^2 \qquad (\delta = 1)$$

TUR Derivation for Markov Jump Process

What perturbation leads to these?

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

$$\boxed{\begin{array}{l} \to \partial_\epsilon \langle\Theta\rangle_\epsilon|_{\epsilon=0} = \langle\Theta\rangle \\ \to \mathcal{I}(0) = \dfrac{\langle\Sigma\rangle}{2k_{\mathrm{B}}} \end{array}}$$

$\to$ these are satisfied.

In a steady state:

$\to$ perturbed dynamics: $\dot{p}_x = \sum_{y(\neq x)} \left[R^\epsilon_{xy} p_y - R^\epsilon_{yx} p_x \right]$

$$\eta_{xy} \equiv \frac{2R_{yx}p_x^{\mathrm{ss}}}{R_{xy}p_y^{\mathrm{ss}} + R_{yx}p_x^{\mathrm{ss}}}$$

$R^\epsilon_{xy} = [1 + \epsilon(1 - \eta_{xy}\delta)]R_{xy}$ $\quad \delta = 0$ or 1

Fisher information

$$\mathcal{I}(0) = \int_0^\tau dt \underbrace{\sum_{x\neq y} R_{xy}p_y^{\mathrm{ss}}}_{= \dot{A}(t)\,:\ \text{dynamical activity}} = A(\tau) \qquad (\delta = 0)$$

$$= \int_0^\tau dt \sum_{x\neq y} R_{xy}p_y^{\mathrm{ss}} \underbrace{\left(\frac{R_{xy}p_y^{\mathrm{ss}} - R_{yx}p_x^{\mathrm{ss}}}{R_{xy}p_y^{\mathrm{ss}} + R_{yx}p_x^{\mathrm{ss}}} \right)^2}_{= B_{xy} = B_{yx}} \qquad (\delta = 1)$$

$$= \int_0^\tau dt \left(\sum_{x>y} R_{xy}p_y^{\mathrm{ss}} B_{xy} + \sum_{x<y} R_{xy}p_y^{\mathrm{ss}} \underbrace{B_{xy}}_{= B_{yx}} \right) = \int_0^\tau dt \left(\sum_{x>y} R_{xy}p_y^{\mathrm{ss}} B_{xy} + \sum_{x>y} R_{yx}p_x^{\mathrm{ss}} B_{xy} \right)$$

$$= \int_0^\tau dt \sum_{x>y} (R_{xy}p_y^{\mathrm{ss}} + R_{yx}p_x^{\mathrm{ss}}) B_{xy} = \int_0^\tau dt \sum_{x>y} \frac{(R_{xy}p_y^{\mathrm{ss}} - R_{yx}p_x^{\mathrm{ss}})^2}{R_{xy}p_y^{\mathrm{ss}} + R_{yx}p_x^{\mathrm{ss}}}$$

TUR Derivation for Markov Jump Process

What perturbation leads to these?

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

$$\boxed{\begin{array}{l} \to \partial_\epsilon \langle \Theta \rangle_\epsilon |_{\epsilon=0} = \langle \Theta \rangle \\ \to \mathcal{I}(0) = \dfrac{\langle \Sigma \rangle}{2k_B} \end{array}}$$

$\to$ these are satisfied.

In a steady state:

$\to$ perturbed dynamics: $\dot{p}_x = \sum_{y(\neq x)} \left[R^\epsilon_{xy} p_y - R^\epsilon_{yx} p_x \right]$

$$\eta_{xy} \equiv \frac{2R_{yx}p_x^{ss}}{R_{xy}p_y^{ss} + R_{yx}p_x^{ss}}$$

$$R^\epsilon_{xy} = [1+\epsilon(1-\eta_{xy}\delta)]R_{xy} \quad \delta = 0 \text{ or } 1$$

Fisher information

$$\mathcal{I}(0) = \int_0^\tau dt \underbrace{\boxed{\sum_{x\neq y} R_{xy} p_y^{ss}}}_{= \dot{A}(t)\,:\ \text{dynamical activity}} = A(\tau) \qquad (\delta = 0)$$

$$= \int_0^\tau dt \sum_{x>y} \frac{(R_{xy}p_y^{ss} - R_{yx}p_x^{ss})^2}{R_{xy}p_y^{ss} + R_{yx}p_x^{ss}} \equiv \frac{1}{2k_B}\langle \Sigma_{ps} \rangle \qquad (\delta = 1)$$

$$\leq \frac{1}{2}\int_0^\tau dt \sum_{x>y} (R_{xy}p_y^{ss} - R_{yx}p_x^{ss}) \ln \frac{R_{xy}p_y^{ss}}{R_{yx}p_x^{ss}} = \frac{1}{2}\int_0^\tau dt \underbrace{\boxed{\sum_{x\neq y} R_{xy}p_y^{ss} \ln \frac{R_{xy}p_y^{ss}}{R_{yx}p_x^{ss}}}}_{= \langle \dot{\Sigma} \rangle / k_B} = \frac{1}{2k_B}\langle \Sigma^{ss} \rangle$$

$$\underbrace{\frac{a-b}{\ln a - \ln b}}_{\text{log mean}} \leq \underbrace{\frac{a+b}{2}}_{\text{arithmatic mean}} \quad \to \frac{(a-b)^2}{a+b} \leq \frac{1}{2}(a-b)\ln\frac{a}{b}$$

TUR Derivation for Markov Jump Process

What perturbation leads to these?

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

$$\boxed{\begin{aligned}&\to \partial_\epsilon \langle\Theta\rangle_\epsilon\big|_{\epsilon=0} = \langle\Theta\rangle \\ &\to \mathcal{I}(0) = \frac{\langle\Sigma\rangle}{2k_B}\end{aligned}}$$

$\to$ these are satisfied.

In a steady state:

$\to$ perturbed dynamics: $\dot{p}_x = \sum_{y(\neq x)} \left[R^\epsilon_{xy} p_y - R^\epsilon_{yx} p_x\right]$

$$\eta_{xy} \equiv \frac{2R_{yx}p_x^{ss}}{R_{xy}p_y^{ss} + R_{yx}p_x^{ss}}$$

$$R^\epsilon_{xy} = [1 + \epsilon(1 - \eta_{xy}\delta)]R_{xy} \quad \delta = 0 \text{ or } 1$$

Fisher information

$$\mathcal{I}(0) = \int_0^\tau dt \underbrace{\boxed{\sum_{x\neq y} R_{xy} p_y^{ss}}}_{= \dot{A}(t)\,:\ \text{dynamical activity}} = A(\tau) \qquad (\delta = 0)$$

$$= \int_0^\tau dt \sum_{x>y} \frac{(R_{xy}p_y^{ss} - R_{yx}p_x^{ss})^2}{R_{xy}p_y^{ss} + R_{yx}p_x^{ss}} \equiv \frac{1}{2k_B}\langle\Sigma_{ps}\rangle \leq \frac{1}{2k_B}\langle\Sigma^{ss}\rangle \qquad (\delta = 1)$$

Cramér-Rao

$$\frac{\mathrm{Var}_\epsilon[\Theta]\big|_{\epsilon=0}}{\left(\partial_\epsilon\langle\Theta\rangle_\epsilon\big|_{\epsilon=0}\right)^2} \geq \frac{1}{\mathcal{I}(0)} \Rightarrow \frac{\mathrm{Var}[\Theta]}{\langle\Theta\rangle^2} A(\tau) \geq 1 \qquad (\delta = 0)$$

Kinetic Uncertainty Relation

$$\frac{\mathrm{Var}[\Theta]}{\langle\Theta\rangle^2}\langle\Sigma^{ss}\rangle \geq \frac{\mathrm{Var}[\Theta]}{\langle\Theta\rangle^2}\langle\Sigma_{ps}\rangle \geq 2k_B \qquad (\delta = 1)$$

TUR

TUR and Variants of TUR

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

$$\frac{\mathrm{Var}[\Theta]}{\langle\Theta\rangle^2}\langle\Sigma\rangle \geq 2k_\mathrm{B}$$ (steady state)

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

Steady-state KUR (Markov jump process)

$$\frac{\mathrm{Var}[\Theta]}{\langle\Theta\rangle^2}A(\tau) \geq 1$$ (steady state)

Terlizzi and Baiesi, J Phys A 52, 02LT03 (2019)

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

$$\frac{\mathrm{Var}[\Theta]}{(\hat{h}_\mathrm{o}\langle\Theta\rangle)^2}\langle\Sigma\rangle \geq 2k_\mathrm{B}$$ (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)

$$\frac{\mathrm{Var}[\Theta]}{(\hat{h}_\mathrm{u}\langle\Theta\rangle)^2}\left(\langle\Sigma\rangle + I\right) \geq 2k_\mathrm{B}$$ (arbitrary time-dependent protocol)

Lee, Park, Park, PRE 104, L052102 (2021)

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

I : related to initial shannon entropy

Application of TUR

1. Estimation of entropy production

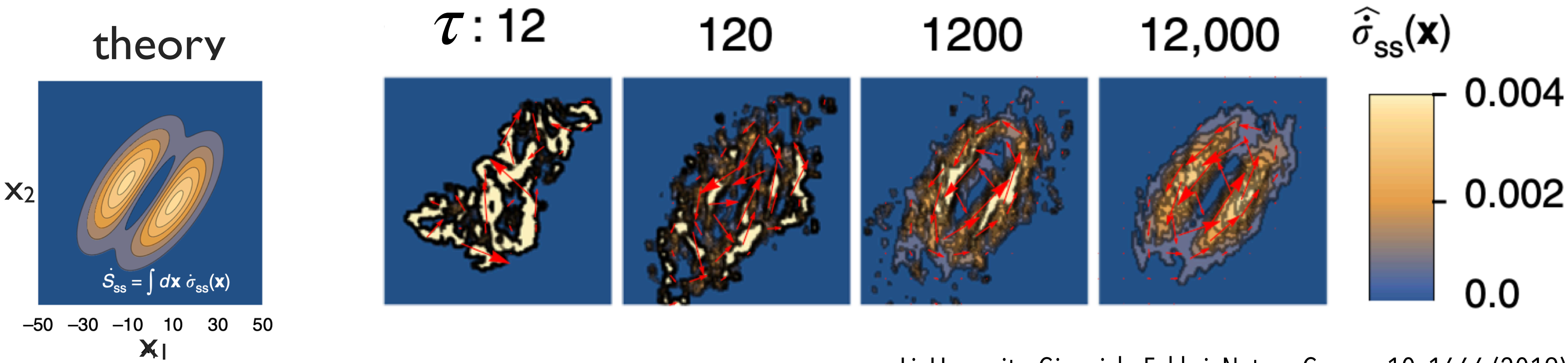
1) direct measurement of path probability

$$R \equiv \ln \frac{p_0(z_0)\mathscr{P}(\Gamma \mid z_0)}{p_\tau(z_\tau)\tilde{\mathscr{P}}(\tilde{\Gamma} \mid \tilde{z}_\tau)}$$: not feasible to measure path probability

2) direct measurement from $P(\mathbf{x}),\ J(\mathbf{x})$

$$\langle \dot{\Sigma} \rangle = \int d\mathbf{x}\, \frac{J(\mathbf{x})\mathsf{D}^{-1}J(\mathbf{x})}{P(\mathbf{x})} \qquad P(\mathbf{x}) = \frac{1}{\tau}\int_0^\tau \delta(\mathbf{x}(t)-\mathbf{x})dt \qquad J(\mathbf{x}) = \frac{1}{\tau}\int_0^\tau \delta(\mathbf{x}(t)-\mathbf{x})\circ d\mathbf{x}$$

(It takes long time, and not feasible for high dimensional systems)



Li, Horowitz, Gingrich, Fakhri, Nature Comm. 10, 1666 (2019)

Application of TUR

1. Estimation of entropy production

3) using TUR $\langle \Sigma \rangle \geq 2 \dfrac{\langle \Theta \rangle^2}{\langle \Theta^2 \rangle - \langle \Theta \rangle^2} \equiv B[\Theta]$

- pros: experimentally feasible (measurable current)
- cons: not exact, but bound
- study to find Θ_{max} which makes B maximum: tightest
- condition for satisfying $B[\Theta_{\max}] = \langle \Sigma \rangle$

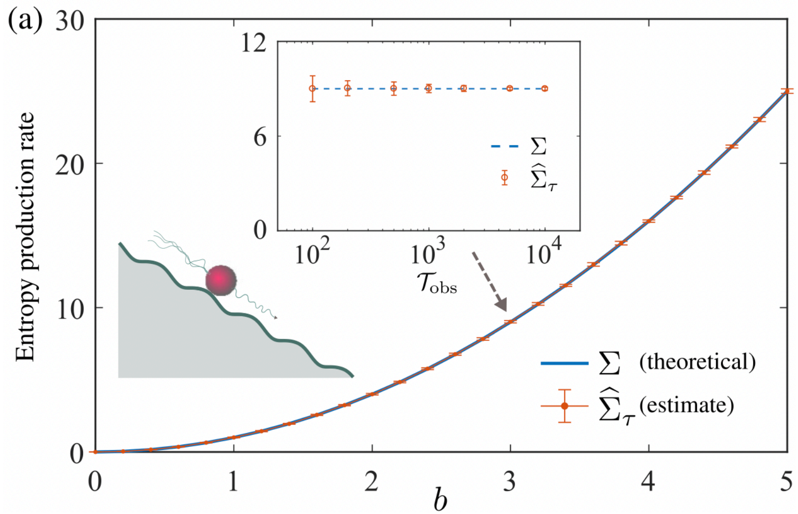
a. short time and $\Theta_{max} = \Sigma$ Manikandan, Gupta, Krishnamurth, PRL 124, 120603 (2020)

b. multiple observables $\Theta_1, \Theta_2, \Theta_3, \ldots \rightarrow \sum_n a_n \Theta_n \approx \Sigma$

Multidimensional TUR method

Dechant, J Phys A 52, 035001 (2018)

Dechant and Sasa, PRX 11, 041061 (2021)



periodically driven particle

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

c. multidimensional entropic bound Lee et al., arXiv:2207.05961

Application of TUR

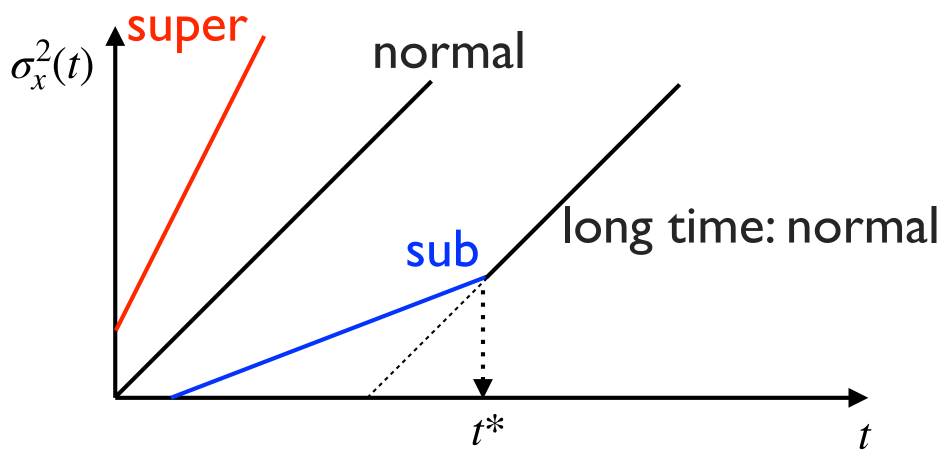
2. Estimation of extent of anomalous diffusion

Hartich and Godec, PRL 127, 080601 (2021)

- anomalous diffusion:

$\langle x_t \rangle = vt$ (driven)

$$\sigma_x^2(t) \equiv \langle x_t^2 \rangle - \langle x_t \rangle^2 \simeq K t^{\alpha} \begin{cases} \alpha > 1 & \text{super} \\ \alpha = 1 & \text{normal} \\ \alpha < 1 & \text{sub} \end{cases}$$

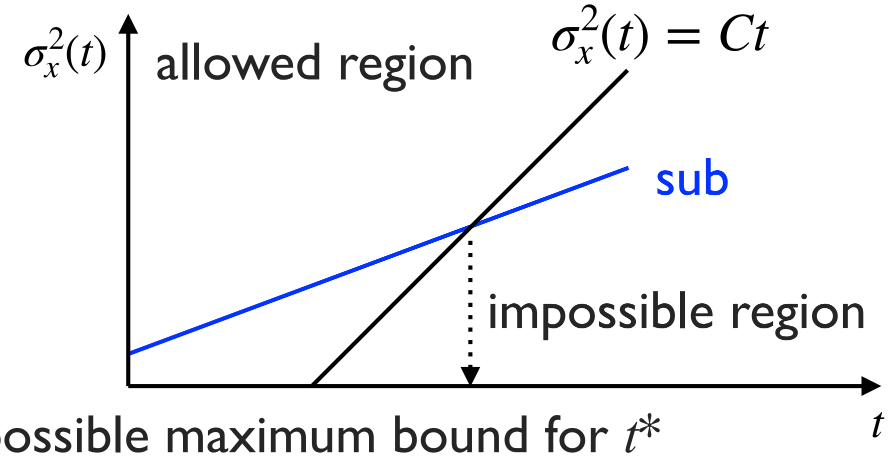


- possible to estimate t^* ?

- TUR: $\dfrac{\sigma_x^2(t)}{\langle x_t \rangle^2} \langle \Sigma \rangle \geq 2k_B$

$$\langle x_t \rangle^2 = v^2 t^2, \quad \langle \Sigma \rangle = \frac{\dot{W} t}{T}$$

$$\sigma_x^2(t) \geq Ct \quad \left(C = \frac{2k_B T v^2}{\dot{W}} \right)$$



possible maximum bound for t^*

Application of TUR

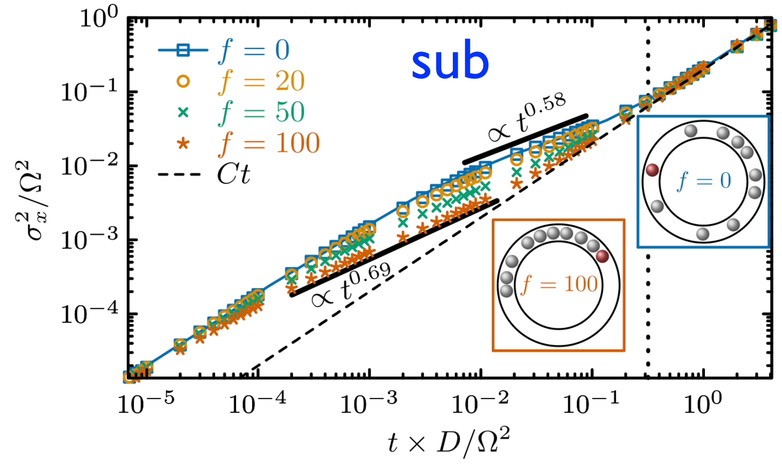
2. Estimation of extent of anomalous diffusion

Hartich and Godec, PRL 127, 080601 (2021)

- anomalous diffusion:

$$\langle x_t \rangle = vt \quad \text{(driven)}$$

$$\sigma_x^2(t) \equiv \langle x_t^2 \rangle - \langle x_t \rangle^2 \simeq K t^\alpha \begin{cases} \alpha > 1 & \text{super} \\ \alpha = 1 & \text{normal} \\ \alpha < 1 & \text{sub} \end{cases}$$



- possible to estimate t^* ?

- TUR: $$\frac{\sigma_x^2(t)}{\langle x_t \rangle^2} \langle \Sigma \rangle \geq 2k_B$$

$$\downarrow \quad \langle x_t \rangle^2 = v^2 t^2, \quad \langle \Sigma \rangle = \frac{\dot{W} t}{T}$$

$$\sigma_x^2(t) \geq Ct \quad \left(C = \frac{2k_B T v^2}{\dot{W}} \right)$$