Bounds on the power spectral density (arXiv: 2306.00417)

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Thermodynamic inequalities in frequency space

- recent years: many new types of thermodynamic inequalities
  - thermodynamic uncertainty relation: statistics of current $\leftrightarrow$ entropy production
    [Barato & Seifert, PRL 2015]
  - thermodynamic speed limit: process time $\leftrightarrow$ entropy production and activity
    [Shiraishi, Funo & Saito, PRL 2018]
- thermodynamic inequalities provide constraints on observable phenomena
- bounds on observables in time space: $J(t)$, $d(p_\tau, p_0)$
- can we derive bounds on observables in frequency space?

Basic concepts and main results

Power spectral density

- fundamental quantity in frequency space: power spectral density (PSD)
- noisy dynamics in steady state
- time trace of observable $z(t)$, $t \in [0, \tau]$

$$Z(\omega, \tau) = \int_0^\tau dt \; e^{i\omega t} z(t) \qquad \text{finite-time Fourier transform}$$

- PSD defined as long-time limit of variance

$$S^z(\omega) = \lim_{\tau \to \infty} \frac{1}{\tau} \text{Var}(Z(\omega, \tau)).$$

Properties of PSD

- Wiener-Khinchine theorem: PSD ⇔ autocorrelation

$$S^z(\omega) = \int_{-\infty}^{\infty} dt\ e^{i\omega t}\mathsf{Cov}(z(t), z(0)).$$

- density of fluctuations in frequency space

$$\frac{1}{\pi}\int_0^{\infty} d\omega\ S^z(\omega) = \mathsf{Var}_{\mathsf{st}}(z) \quad \Rightarrow \quad \frac{1}{\pi}\int_{\omega}^{\omega+\Delta\omega} S^z(\omega) = \text{“power” contained in } [\omega, \omega+\Delta\omega]$$

- low- and high-frequency limit: long- and short-time fluctuations

$$\lim_{\omega\to 0} S^z(\omega) = \lim_{\tau\to\infty} \tau\mathsf{Var}(\bar{z}_\tau) \qquad \bar{z}_\tau = \frac{1}{\tau}\int_0^{\tau} dt\ z(t)$$

$$\lim_{\omega\to\infty} \omega^2 S^z(\omega) = \lim_{dt\to 0} \frac{\mathsf{Var}(dz)}{dt} \qquad dz = z(t+dt) - z(t)$$

Concrete example: diffusive dynamics

- overdamped Langevin equation ⇔ Fokker-Planck equation

$$\dot{\boldsymbol{x}}(t) = \boldsymbol{a}(\boldsymbol{x}(t)) + \boldsymbol{G}\boldsymbol{\xi}(t), \qquad \boldsymbol{B} = \frac{1}{2}\boldsymbol{G}\boldsymbol{G}^{\mathsf{T}}$$

$$\Rightarrow \qquad 0 = -\boldsymbol{\nabla}\big(\boldsymbol{\nu}_{\mathsf{st}}(\boldsymbol{x})p_{\mathsf{st}}(\boldsymbol{x})\big), \qquad \boldsymbol{\nu}_{\mathsf{st}}(\boldsymbol{x}) = \boldsymbol{a}(\boldsymbol{x}) - \boldsymbol{B}\boldsymbol{\nabla}_x \ln p_{\mathsf{st}}(\boldsymbol{x})$$

- detailed balance: $\boldsymbol{a}(\boldsymbol{x}) = \boldsymbol{B}\boldsymbol{\nabla}\psi(\boldsymbol{x}) \Rightarrow p_{\mathsf{st}}(\boldsymbol{x}) \propto e^{-\psi(\boldsymbol{x})}$, $\boldsymbol{\nu}_{\mathsf{st}}(\boldsymbol{x}) = 0$
- in general: irreversible flows $\boldsymbol{\nu}_{\mathsf{st}}(\boldsymbol{x}) \neq 0 \Rightarrow$ non-equilibrium steady state

$$\sigma_{\mathsf{st}} = \int d\boldsymbol{x}\ \boldsymbol{\nu}_{\mathsf{st}}(\boldsymbol{x})\boldsymbol{B}^{-1}\boldsymbol{\nu}_{\mathsf{st}}(\boldsymbol{x})p_{\mathsf{st}}(\boldsymbol{x}) \geq 0 \qquad \text{entropy production rate}$$

- observable: arbitrary configuration-dependent function $z(\boldsymbol{x}) \Rightarrow z(t) = z(\boldsymbol{x}(t))$

Variational expression for PSD

- central result: variational formula for PSD

$$S^z(\omega) = 2 \sup_\chi \inf_\eta \Big[2\Re\big(\mathrm{Cov}_{\mathrm{st}}(z + \boldsymbol{\nu}_{\mathrm{st}} \boldsymbol{\nabla} \eta - i\omega\eta, \chi^*)\big) + \langle \boldsymbol{\nabla}\eta^* \boldsymbol{B} \boldsymbol{\nabla}\eta \rangle_{\mathrm{st}} - \langle \boldsymbol{\nabla}\chi^* \boldsymbol{B} \boldsymbol{\nabla}\chi \rangle_{\mathrm{st}} \Big]$$

$$\chi(\boldsymbol{x}), \eta(\boldsymbol{x}) \in \mathbb{C} \text{ differentiable functions}$$

- in equilibrium: $\boldsymbol{\nu}_{\mathrm{st}}(\boldsymbol{x}) = 0$

$$S^z_{\mathrm{eq}}(\omega) = \sup_\chi \inf_\eta \left[\frac{\mathrm{Cov}_{\mathrm{st}}(z,\chi)^2}{\langle \boldsymbol{\nabla}\chi \boldsymbol{B} \boldsymbol{\nabla}\chi \rangle_{\mathrm{st}} + \omega^2 \frac{\mathrm{Cov}_{\mathrm{st}}(\eta,\chi)^2}{\langle \boldsymbol{\nabla}\eta \boldsymbol{B} \boldsymbol{\nabla}\eta \rangle_{\mathrm{st}}}} \right], \qquad \chi(\boldsymbol{x}), \eta(\boldsymbol{x}) \in \mathbb{R}$$

- variational expression difficult to evaluate explicitly
- useful as starting point for deriving bounds on PSD

Bounds on PSD

- specific choice of $\eta(\boldsymbol{x})/\chi(\boldsymbol{x}) \Rightarrow$ lower/upper bound on PSD
- lower and upper bound expressed in terms of two parameters: C^0 and C^∞

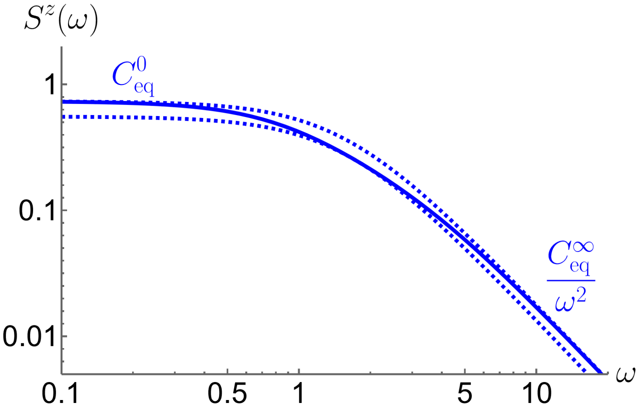
$$\frac{1}{C^\infty + \omega^2 C^0} \leq \frac{S^z(\omega)}{2\mathsf{Var}_{\mathsf{st}}(z)} \leq \frac{1}{\frac{1}{C^0} + \frac{\omega^2}{C^\infty}}$$

- in equilibrium: low- and high-frequency limit of PSD!

$$C^0 = \frac{\lim_{\omega \rightarrow 0} S^z_{\mathsf{eq}}(\omega)}{2\mathsf{Var}_{\mathsf{st}}(z)}, \qquad C^\infty = \frac{\lim_{\omega \rightarrow \infty} \omega^2 S^z_{\mathsf{eq}}(\omega)}{2\mathsf{Var}_{\mathsf{st}}(z)}$$

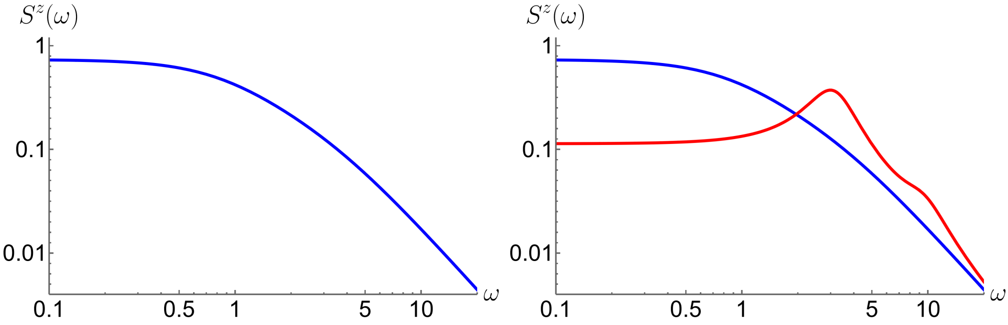
- equilibrium PSD at any frequency bounded by asymptotic behavior
- upper bound tight and low and high frequencies

Bounds on PSD in equilibrium



PSD in and out of equilibrium

- in equilibrium: PSD monotonically decaying function of ω (eigenvalues of generator real)



- out of equilibrium: generator can have complex eigenvalues $\lambda \in \mathbb{C}$
  $\Rightarrow$ peaks in PSD at $\omega = |\Im(\lambda)|$, width $\Re(\lambda)$

Bounds on PSD out of equilibrium

- out of equilibrium: C^∞ modified by presence of flows

$$C^0 = \sup_{\chi \in \mathbb{R}} \left[\frac{\mathsf{Cov}_{\mathsf{st}}(z,\chi)^2}{\mathsf{Var}_{\mathsf{st}}(z) \left\langle \boldsymbol{\nabla}\chi \boldsymbol{B} \boldsymbol{\nabla}\chi \right\rangle_{\mathsf{st}}} \right] = \frac{\lim_{\omega \to 0} S^z_{\mathsf{eq}}(\omega)}{2\mathsf{Var}_{\mathsf{st}}(z)}$$

$$C^\infty = \frac{\lim_{\omega \to \infty} \omega^2 S^z(\omega)}{2\mathsf{Var}_{\mathsf{st}}(z)} + \sup_{\chi \in \mathbb{R}} \left[\frac{\left\langle \chi \boldsymbol{\nabla} z \boldsymbol{\nu}_{\mathsf{st}} \right\rangle^2_{\mathsf{st}}}{\mathsf{Var}_{\mathsf{st}}(z) \left\langle \boldsymbol{\nabla}\chi \boldsymbol{B} \boldsymbol{\nabla}\chi \right\rangle_{\mathsf{st}}} \right]$$

- $S^z_{\mathsf{eq}}(\omega)$: PSD of equilibrium dynamics with same steady state $p_{\mathsf{st}}(\boldsymbol{x})$
- irreversible flows $\boldsymbol{\nu}_{\mathsf{st}}(\boldsymbol{x}) \Rightarrow$ less strict constraints on PSD

PSD in and out of equilibrium - once more with bounds

- how does PSD change when driving system out of equilibrium?
- compare to equilibrium dynamics with same steady state: $\boldsymbol{a}(\boldsymbol{x}) = \boldsymbol{B}\boldsymbol{\nabla} \ln p_{\text{st}}(\boldsymbol{x})$
- driving reduces zero-frequency component

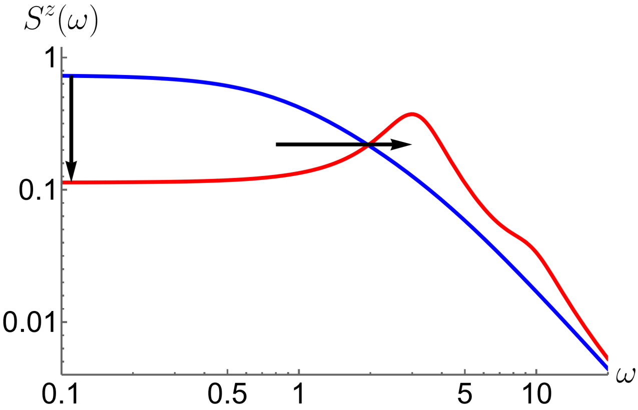
$$S^z(\omega) \leq S^z_{\text{eq}}(0) \qquad \Rightarrow \qquad S^z(0) \leq S^z_{\text{eq}}(0)$$

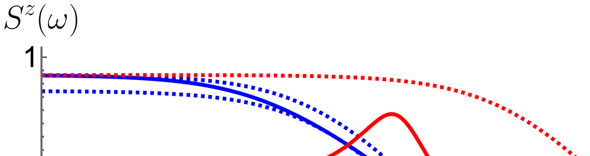
- total power invariant under driving

$$\frac{1}{\pi}\int_0^\infty d\omega\ S^z(\omega) = \text{Var}_{\text{st}}(z) = \frac{1}{\pi}\int_0^\infty d\omega\ S^z_{\text{eq}}(\omega)$$

- driving shifts power to higher frequencies

Bounds on PSD out of equilibrium





Bounds on entropy production

- any upper bound on C^0 and C^∞ $\Rightarrow$ lower and upper bound on PSD

$$C^0 \leq \infty, \qquad C^\infty \leq \frac{\lim_{\omega\to\infty} \omega^2 S^z(\omega)}{2\mathsf{Var}_{\mathsf{st}}(z)} + \frac{\Delta z^2 \sigma_{\mathsf{st}}}{4\mathsf{Var}_{\mathsf{st}}(z)}$$

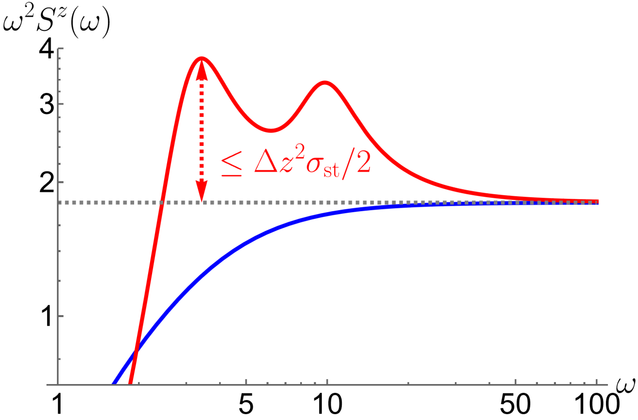
σ_{st} entropy production rate, $\Delta z = z_{\mathsf{max}} - z_{\mathsf{min}}$ range of observable

- rewrite as bound on entropy production

$$\sigma_{\mathsf{st}} \geq \frac{2}{\Delta z^2}\left(\omega^2 S^z(\omega) - \lim_{\omega\to\infty} \omega^2 S^z(\omega)\right)$$

- estimate for entropy production from PSD of time-symmetric observable $z(\boldsymbol{x})$
- right-hand side only depends on measured trajectory data

Bounds on entropy production



Applications

Application 1: Brownian gyrator

- solvable example: linear dynamics in two dimensions "Brownian Gyrator"

$$\dot{x}_1(t) = -\mu k_1 x_1(t) - \mu\gamma k_2 x_2(t) + \sqrt{2\mu T}\xi_1(t)$$
$$\dot{x}_2(t) = \underbrace{-\mu k_2 x_2(t)}_{\text{trapping}} + \underbrace{\mu\gamma k_1 x_1(t)}_{\text{driving}} + \sqrt{2\mu T}\xi_2(t)$$

- steady-state (independent of driving) and local mean velocity

$$p_{\text{st}}(x_1, x_2) = \frac{T}{2\pi\sqrt{k_1 k_2}} \exp\left(- \frac{k_1 x_1^2 + k_2 x_2^2}{2T} \right), \qquad \boldsymbol{\nu}_{\text{st}}(x_1, x_2) = \mu\gamma \begin{pmatrix} -k_2 x_2 \\ k_1 x_1 \end{pmatrix}$$

- linear systems → explicit expression for PSD

Application 1: Brownian gyrator

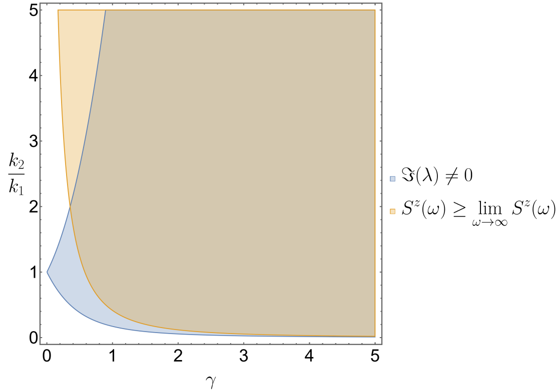
- observable: x_1 coordinate, $z(x_1, x_2) = x_1$
- can we tell whether the system is out of equilibrium by measuring only $x_1(t)$?
- path probability of $\hat{x}_1 = (x_1(t))_{t \in [0,\tau]}$ time-reversal symmetric

$$\Sigma = D_{\mathsf{KL}}\big(\mathbb{P}(\hat{\boldsymbol{x}}) \| \mathbb{P}(\hat{\boldsymbol{x}}^\dagger)\big) \geq D_{\mathsf{KL}}\big(\mathbb{P}(\hat{x}_1) \| \mathbb{P}(\hat{x}_1^\dagger)\big) = 0$$

- no currents in one dimension $\rightarrow$ cannot use TUR
- use spectral properties
  - peaks in PSD $\rightarrow$ oscillations $\rightarrow$ complex eigenvalues $\rightarrow$ out of equilibrium
  - equilibrium systems $\omega^2 S^z(\omega) \leq \lim_{\omega \to \infty} \omega^2 S^z(\omega)$ $\rightarrow$ violation $\rightarrow$ out of equilibrium

Application 1: Brownian gyrator

- condition for complex eigenvalues: $|\gamma| \geq \frac{|k_1 - k_2|}{2\sqrt{k_1 k_2}}$
- condition for violation of PSD bound: $|\gamma| \geq \frac{k_1}{\sqrt{k_2^2 + 2 k_1 k_2}}$
- quantitative estimate on entropy production possible



Application 2: equilibrium fluctuations

- one-dimensional equilibrium diffusion in potential $U(x) = \kappa|x|$
- analytic expression for PSD [Caughey & Dienes, 1961]

$$S^x(\omega) = \frac{2D}{\omega^2}\left[1 + \frac{(\mu\kappa)^4}{4D^2\omega^2}\left(2 - \sqrt{2 + 2\sqrt{1 + \frac{16D^2\omega^2}{(\mu\kappa)^4}}}\right)\right] \qquad D = \mu T$$

- three different measures of fluctuations

$$\mathrm{Var}(x(t+dt)) - x(t)) \simeq 2\mu T dt, \qquad \mathrm{Var}_{\mathrm{st}}(x) = \frac{2T^2}{\kappa^2}, \qquad \mathrm{Var}(\bar{x}) \simeq \frac{10T^3}{\mu\kappa^4\tau}$$

$$\leftrightarrow \lim_{\omega\to\infty} \omega^2 S^x(\omega) \qquad \leftrightarrow \int_0^\infty d\omega\ S^x(\omega) \qquad \leftrightarrow \lim_{\omega\to 0} S^x(0)$$

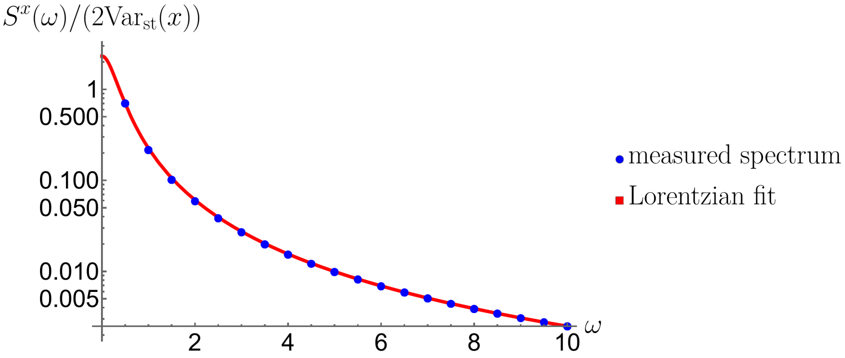
Application 2: equilibrium fluctuations

- in practice: only finite range of frequencies observable
  - time-resolution $\Delta t \rightarrow \omega_{\text{max}} = \frac{\pi}{\Delta t}$
  - measurement time $\tau \rightarrow \omega_{\text{min}} = \frac{\pi}{\tau}$
- how to infer low- and high-frequency behavior?
- high time-resolution but limited observation time $\rightarrow C^\infty = \frac{D}{\text{Var}_{\text{st}}(x)}$ known, $C^0 = ?$
- for $U(x) = \kappa|x|$: $C^0 = \frac{S^x(0)}{2\text{Var}_{\text{st}}(x)} = \frac{5D}{(\mu\kappa)^2}$

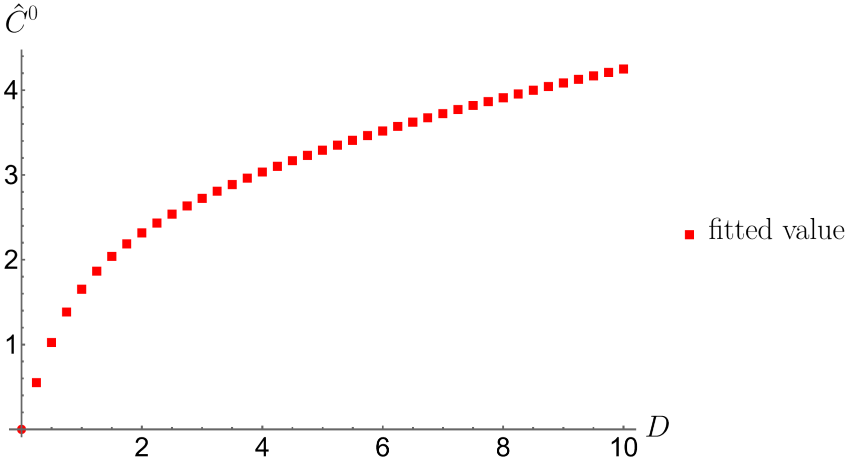
Application 2: equilibrium fluctuations

naive idea: fit power spectrum

$$\frac{\hat{S}^x(\omega)}{2\mathsf{Var}_{\mathsf{st}}(x)} = \frac{1}{\frac{1}{\hat{C}^0} + \frac{\omega^2}{C^\infty}}$$



Application 2: equilibrium fluctuations



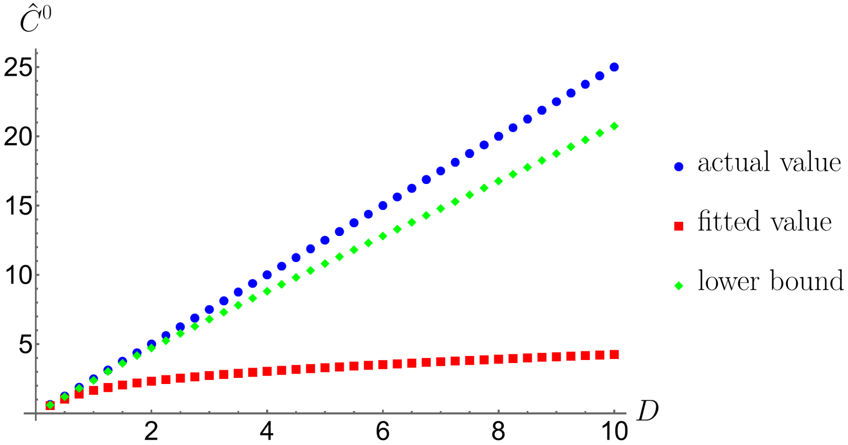
Application 2: equilibrium fluctuations

- alternative approach: use bounds

$$\frac{1}{C^\infty + \omega^2 \hat{C}^0} \leq \frac{S^x(\omega)}{2\mathsf{Var}_{\mathsf{st}}} \leq \frac{1}{\frac{1}{\hat{C}^0} + \frac{\omega^2}{C^\infty}}$$

- two lower bounds on $\hat{C}^0$ for every measurement point of $S^x(\omega)$
- can be used to check consistency of fit results

Application 2: equilibrium fluctuations



$\Rightarrow$ fit describes data, but extrapolated behavior not consistent with bounds!

Concluding remarks

- bounds on PSD in and out of equilibrium
- similar results for Markov jump process
- positive estimate for σ_{st} even when dynamics of $z(\boldsymbol{x})$ are reversible $(\mathbb{P}(\hat{z}^\dagger) = \mathbb{P}(\hat{z}))$
  $\Rightarrow$ characteristic features of non-equilibrium systems beyond time-reversal?
- positive estimate for σ_{st} even for real eigenvalues (no oscillations)
- universal constraint on equilibrium PSD for overdamped and underdamped dynamics
  violation $\Rightarrow$ system out of equilibrium ($\rightarrow$ open quantum systems?)
- use bounds to improve estimates from measured data
  additional information: Markovian dynamics!

Thank you for your attention!

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