

Frequency-resolved fluctuation–response relation as a diagnostic tool for nonequilibrium spectra

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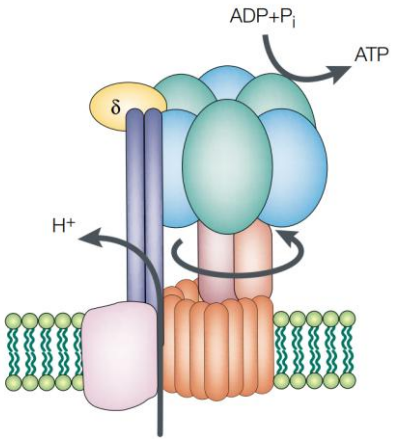
imagine the impossible

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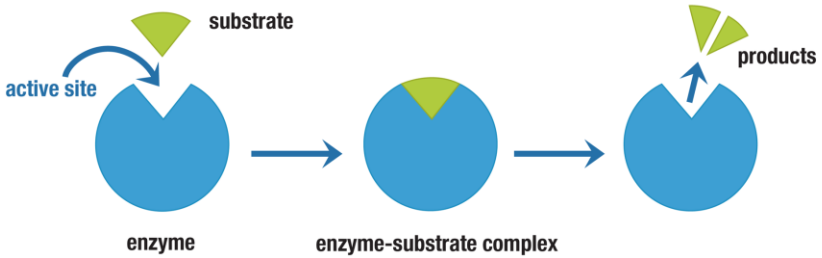
arXiv:2605.05038

Power spectra in nonequilibrium systems

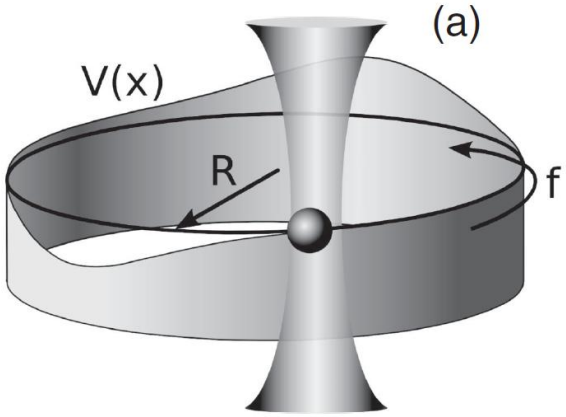
Molecular motors



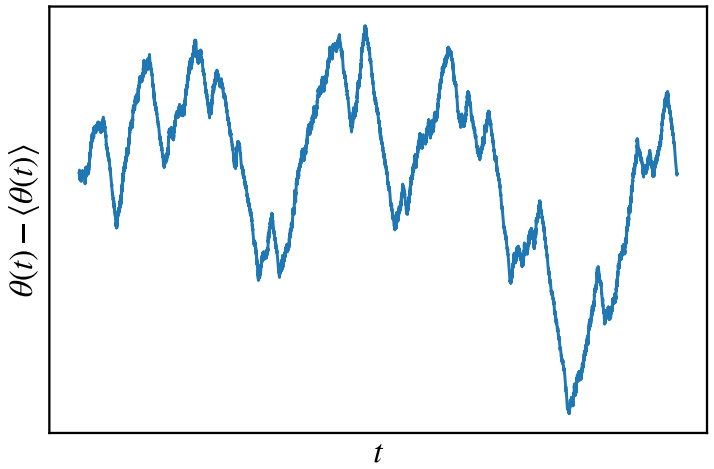
Enzyme kinetics

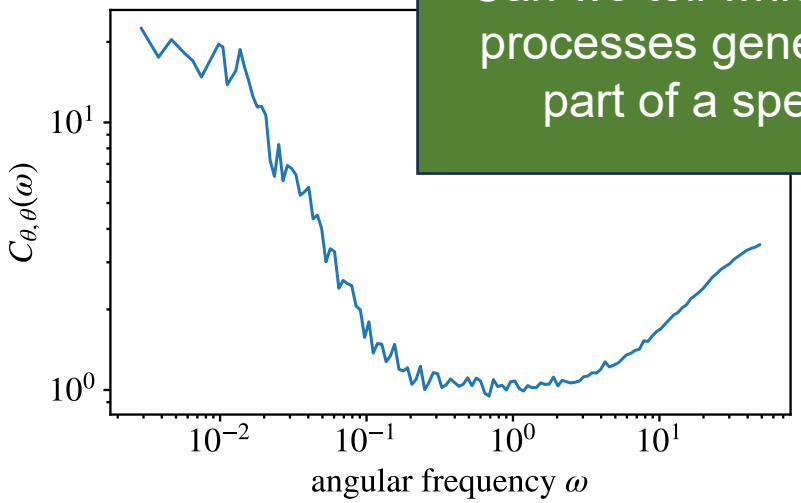


Driven colloidal particle



PRL **98,** 210601 (2007)





Can we tell which physical processes generate each part of a spectrum?

Limitations of FDT and TUR

- How are fluctuation constrained with (thermo)dynamic properties?

Fluctuation-dissipation theorem (FDT)

$$(\text{fluctuation}) = T(\text{response})$$

only applicable to EQ system

Harada–Sasa relation

$$(\text{fluctuation})–T(\text{response}) = (\text{heat dissipation})$$

only applicable to velocity-like observables

Thermodynamic uncertainty relation

$$\frac{(\text{fluctuation})}{(\text{mean current})^2} \geq \frac{1}{(\text{dissipation})}$$

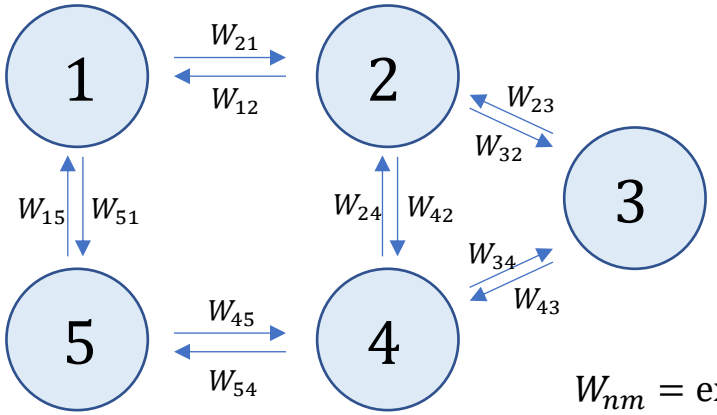
only applicable to time-domain fluctuation

Fluctuation-response relations for frequency domain?

Main result: spectrum decomposition

imagine the impossible
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Markov jump system



$$W_{nm} = \exp\left[B_{nm} + \frac{F_{nm}}{2}\right]$$

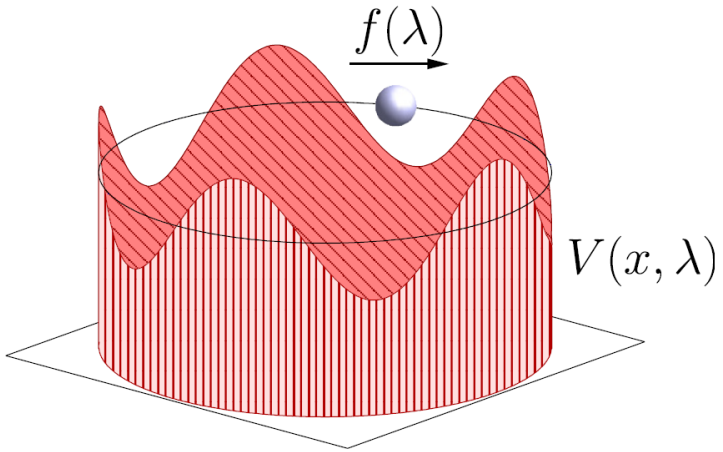
$$\partial_t p_n(t) = \sum_{m(\neq n)} [W_{nm} p_m(t) - W_{mn} p_n(t)]$$

Edge-wise decomposition

$$C_{\theta,\theta}(\omega) = \sum_{e \in \{\text{edges}\}} C^{(e)}_{\theta,\theta}(\omega)$$

$$C^{(e)}_{\theta,\theta}(\omega) = \frac{1}{A^{\phi}_{e}} \left| R^{\theta}_{\phi_e}(\omega) \right|^2$$

Overdamped Langevin system



$$\dot{\boldsymbol{x}}_t = \mathbb{M}(\boldsymbol{x}_t)\boldsymbol{F}(\boldsymbol{x}_t) + \mathbb{B}(\boldsymbol{x}_t) \circledast \boldsymbol{\xi}_t$$

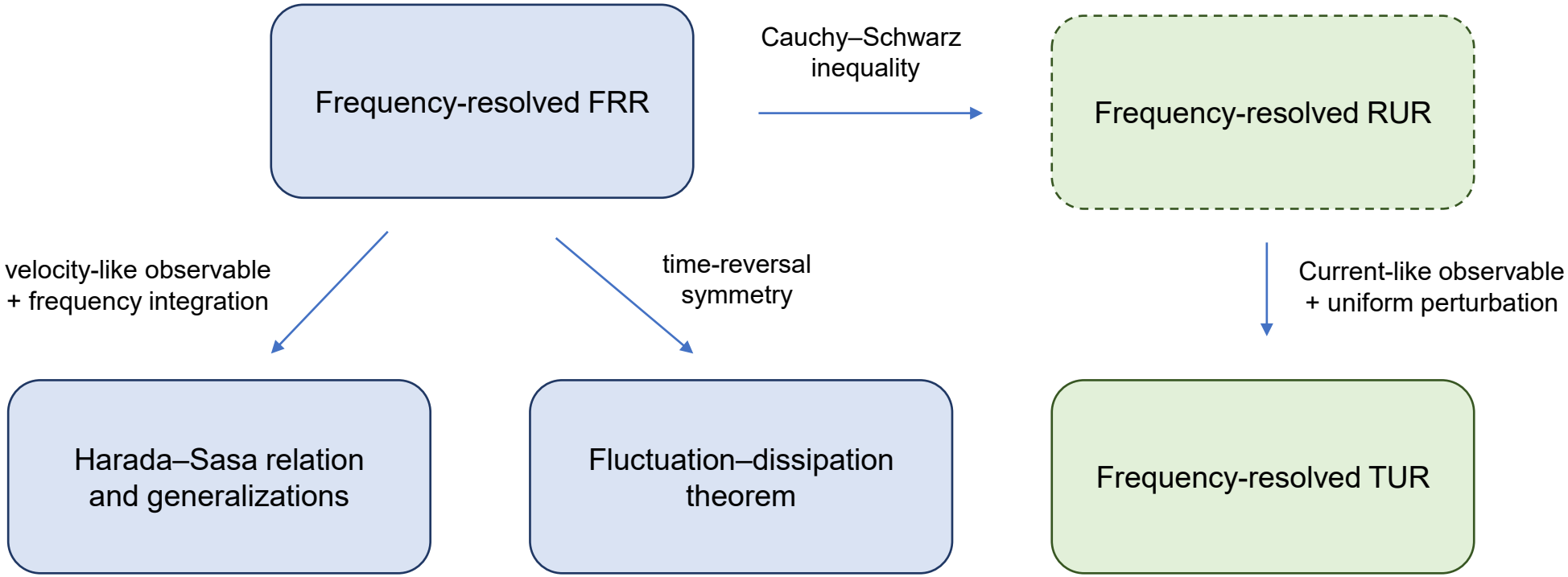
Spatial decomposition

$$C_{\theta,\theta}(\omega) = \sum_{k,l} \int d\boldsymbol{x}\, c_{\theta,\theta}(\boldsymbol{x},\omega)_{kl}$$

$$c_{\theta,\theta}(\boldsymbol{x},\omega)_{kl} = \left[\mathbb{A}^{\phi}(\boldsymbol{x})^{-1}\right]_{kl} R^{\theta}_{\phi_k(\boldsymbol{x})}(\omega) R^{\theta}_{\phi_l(\boldsymbol{x})}(\omega)^*$$

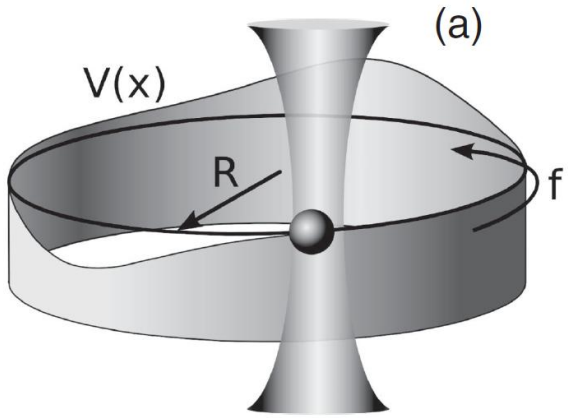
Frequency-resolved fluctuation–response relations (FRR)

Main result: unified hierarchy

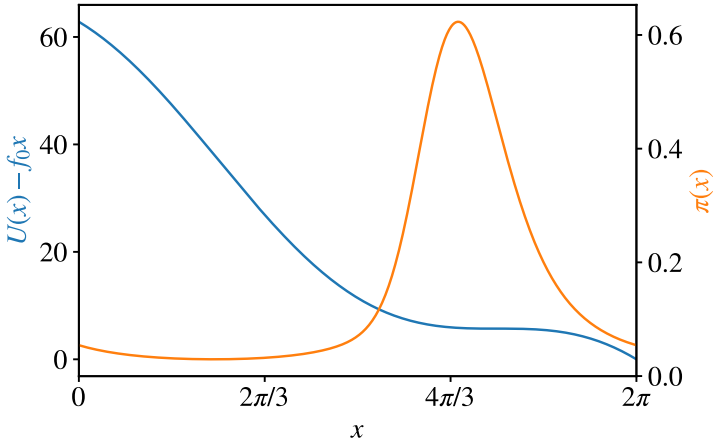


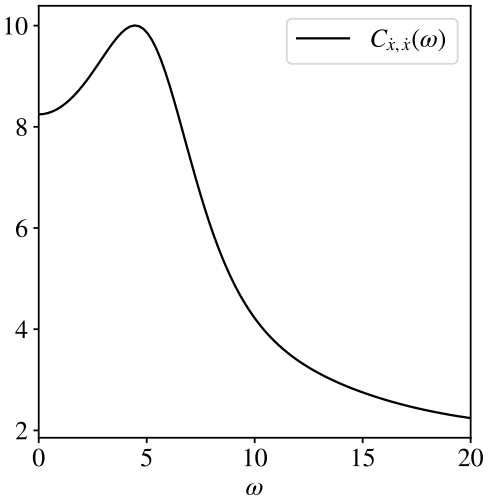
For detailed derivations, see arXiv:2605.05038

Application 1: tilted periodic potential



PRL **98,** 210601 (2007)



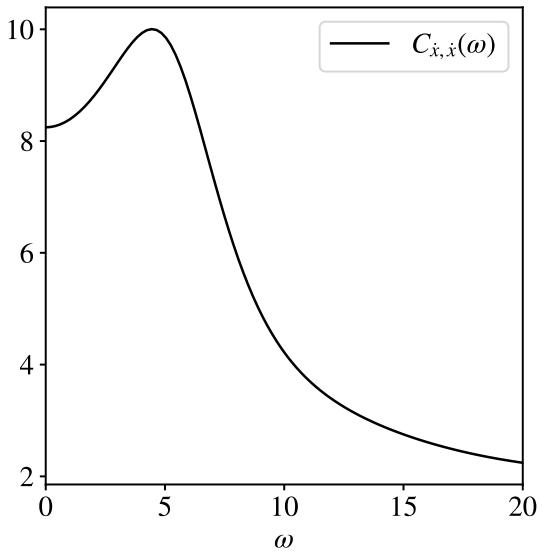


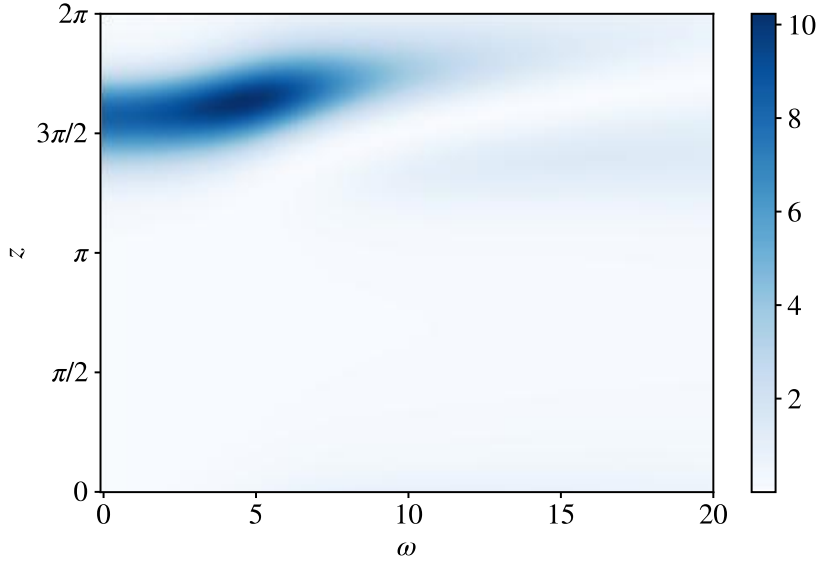
- Overdamped Langevin particle moving on a ring in a tilted periodic potential

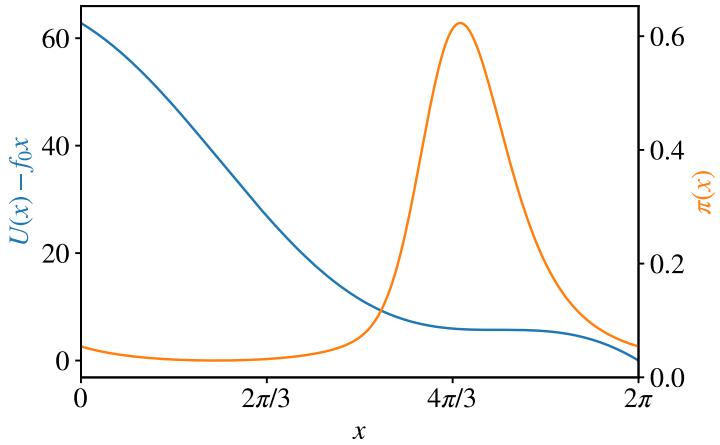
$$\dot{x}(t) = \mu\left[f_0 - U'\left(x(t)\right)\right] + \sqrt{2\mu T}\xi, \qquad U(x) = U_0\cos(2\pi x/L)$$

- For $U_0 = 10, f_0 = 10, L = 2\pi$, we observe a single peak in the PSD of velocity

Application 1: tilted periodic potential

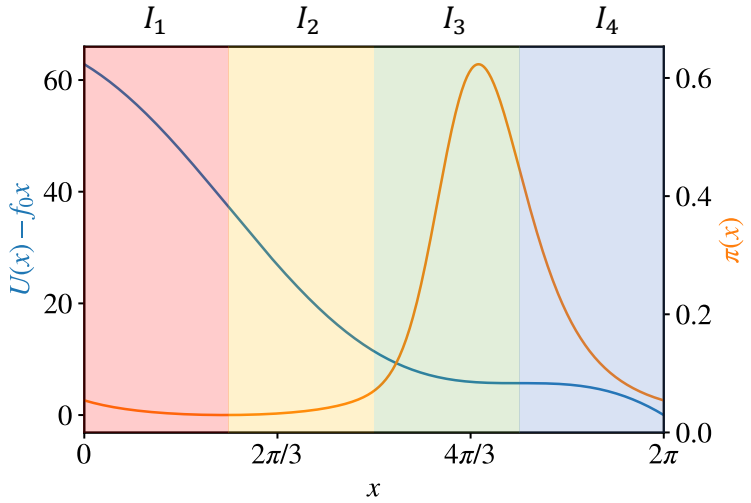


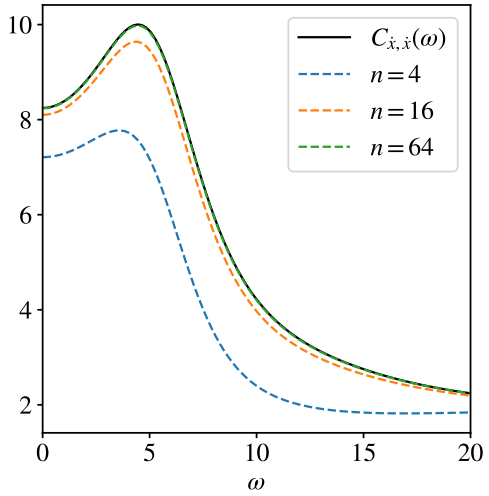




- Spatial decomposition: $C_{\dot{x},\dot{x}}(\omega) = \int_0^L dz c_{\dot{x},\dot{x}}(z,\omega)\,,\ c_{\theta,\theta}(z,\omega) = \frac{2T}{\mu\pi(z)}\left|R^{\dot{x}}_{F(z)}\right|^2$
- $c_{\theta,\theta}(z,\omega)$ quantifies the local contribution of position z to the velocity PSD at frequency ω

Application 1: tilted periodic potential





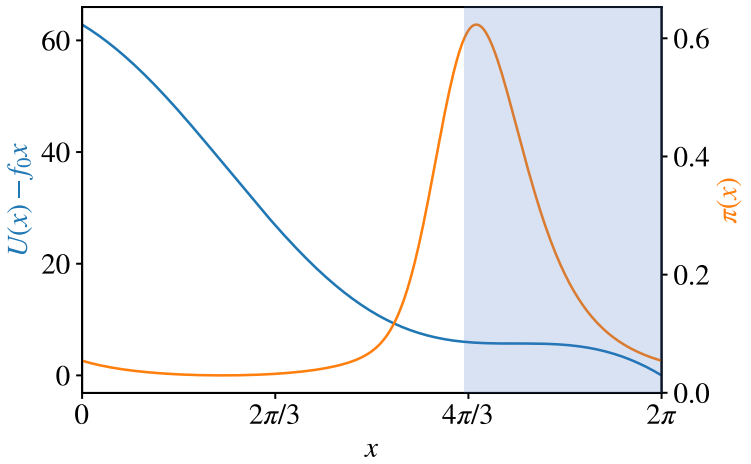
- Pointwise force perturbations are (in most cases) experimentally infeasible
- Coarse-grained version of the FRR

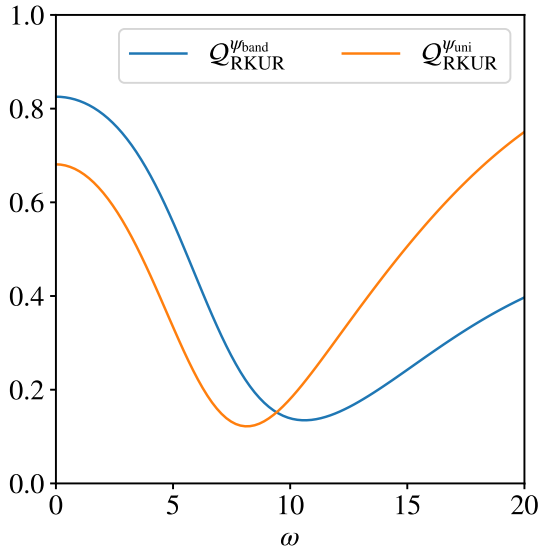
$$C^{(n)}_{\dot{x},\dot{x}}(\omega) = \sum_{i=0}^{n-1} \frac{2T}{\mu} \frac{\left| \int_{I_i} dz\, R^{\dot{x}}_{F(z)}(\omega) \right|^2}{\int_{I_i} dz\, \pi(z)}$$

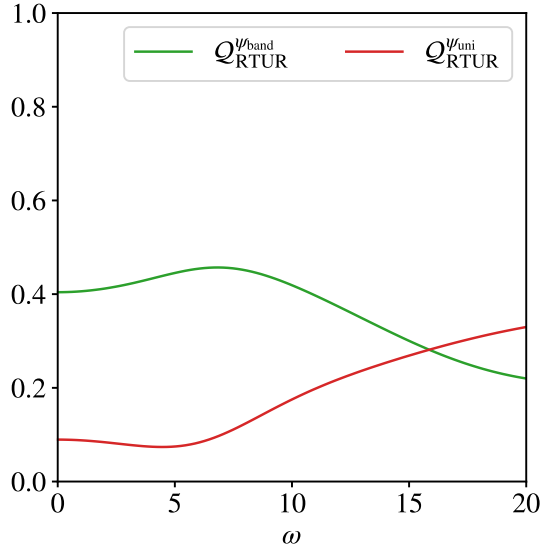
Cauchy–Schwarz
$C^{(n)}_{\dot{x},\dot{x}}(\omega) \leq C_{\dot{x},\dot{x}}(\omega)$

- Even for $n = 4$, the main spectral features are well reproduced
- Local FRR can be implemented with finite spatial resolution

Application 1: tilted periodic potential







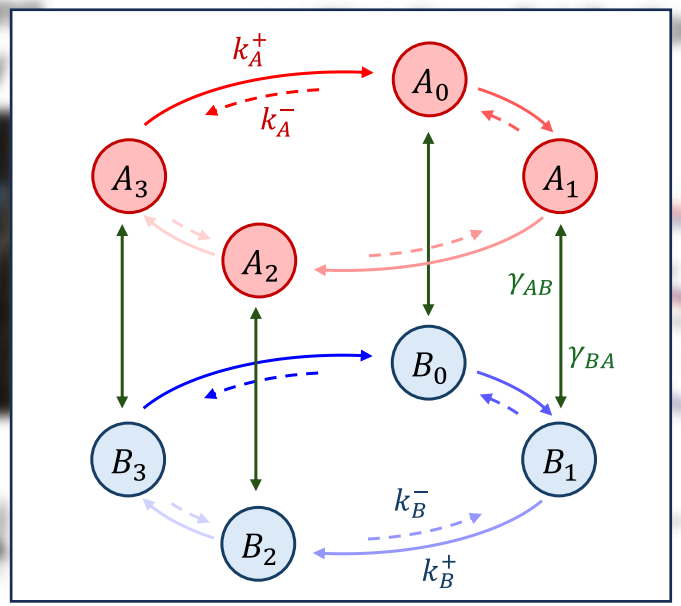
$R^{\dot{x}}_{F,\psi}$: response to $F(x) \mapsto F(x) + \epsilon\psi(x)$

- Frequency-resolved RKUR and RTUR

$$\frac{\left|R^{\dot{x}}_{F,\psi}(\omega)\right|^2}{C_{\dot{x},\dot{x}}(\omega)} \leq \int_0^L dx \frac{\mu\pi(x)}{2T}\psi(x)^2 \quad \text{(RKUR)} \qquad \frac{\left|R^{\dot{x}}_{F,\psi}(\omega)\right|^2}{C_{\dot{x},\dot{x}}(\omega)} \leq \int_0^L dx \frac{j^{\text{ss}}(x)^2}{2\mu T\pi(x)}\psi(x)^2 \quad \text{(RTUR)}$$

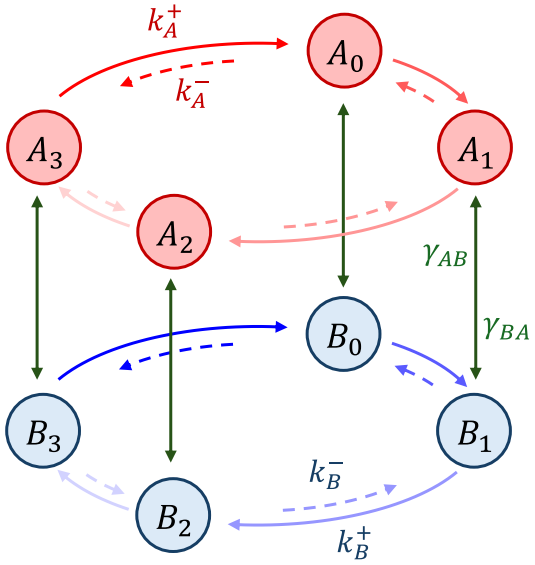
- Uniform perturbation $\psi(x) = 1$ and band perturbation $\psi(x) = 1_{\left[\frac{2L}{3},L\right]}(x)$

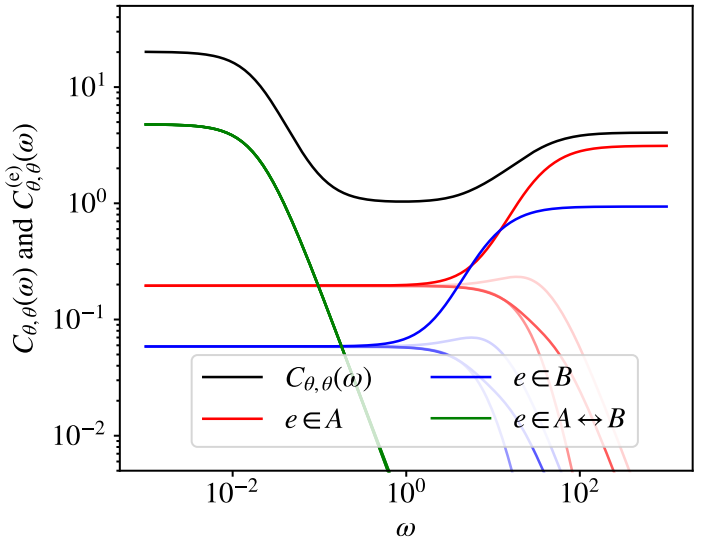
Application 2: dynamic disorder model



- Dynamic disorder: temporal modulation of the apparent transition rates by slowly evolving internal or conformational degrees of freedom
- Very simple model with two conformational states (A and B)
- $k_\alpha^\pm$: rates within a conformation / γ_{AB}, γ_{BA}: transition rates of switching

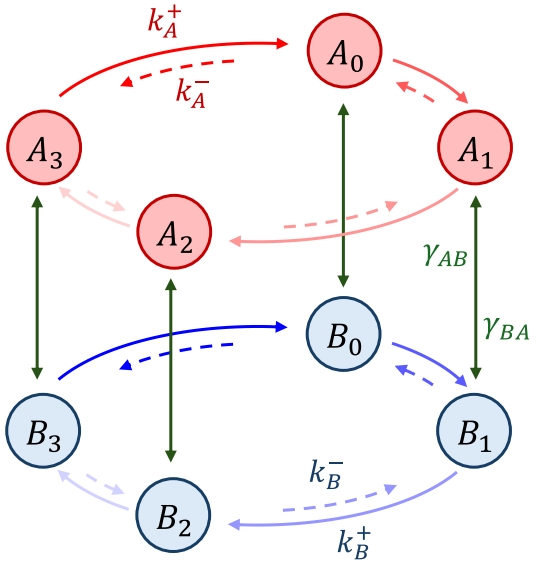
Application 2: dynamic disorder model

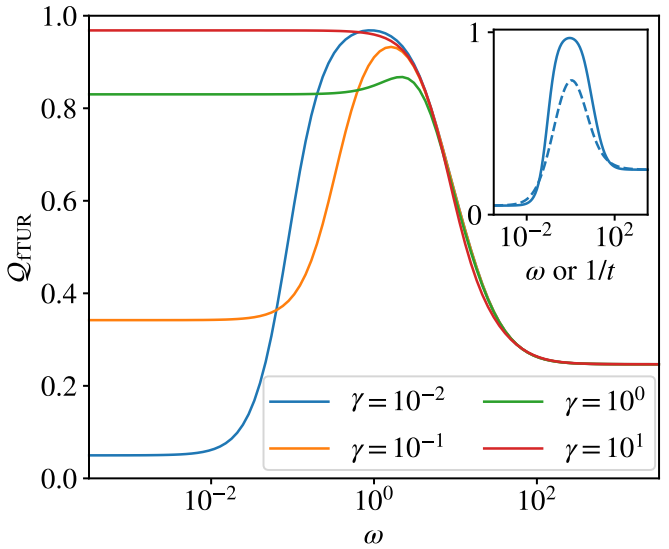




- $\theta(t)$: net instantaneous current through the boundary transitions $(A_3 \to A_0, B_3 \to B_0)$
- $\gamma \ll k$: PSD captures two time scales
- Frequency–resolved FRR: $C_{\theta,\theta}(\omega) = \sum_{e\in\{\text{edges}\}} C_{\theta,\theta}^{(e)}(\omega)\,, \quad C_{\theta,\theta}^{(e)}(\omega) = \left|R_{B_e}^{\theta}\right|^2 / A_e^B$
- Low freq: dominated by switching edge
- High freq: dominated by boundary transitions (fluctuation & response become local)

Application 2: dynamic disorder model





$$\frac{C_{\theta,\theta}(\omega)}{\langle\theta\rangle_{\mathrm{ss}}^2} \geq \frac{2}{\sigma_{\mathrm{tot}}} \quad \text{vs} \quad \frac{C_{\theta,\theta}(t)}{\langle\theta\rangle_{\mathrm{ss}}^2} \geq \frac{2}{\sigma_{\mathrm{tot}}}$$

- Fluctuation-resolved TUR (fTUR)

$$\frac{C_{\theta,\theta}(\omega)}{\langle\theta\rangle_{\mathrm{ss}}^2} \geq \frac{2}{\sigma_{\mathrm{tot}}}$$

- For slow switching, the fTUR becomes tighter at intermediate frequencies
- The finite-time TUR is always looser than the optimized fTUR

Conclusion

- Frequency-resolved FRR decomposes spectra into response channels.
- In Markov jump system systems, the channels are transition edges; in Langevin systems, they are spatial contributions.
- The decomposition helps the understanding of the role of each edge at different frequency
- Frequency-resolved FRR unifies FRR, RUR, TUR, FDT, and Harada–Sasa-type relations.

Edge-wise decomposition

$$C_{\theta,\theta}(\omega) = \sum_{e\in\{\text{edges}\}} C^{(e)}_{\theta,\theta}(\omega)$$

$$C^{(e)}_{\theta,\theta}(\omega) = \frac{1}{A^{\phi}_{e}} \left| R^{\theta}_{\phi_e}(\omega) \right|^2$$

Spatial decomposition

$$C_{\theta,\theta}(\omega) = \sum_{k,l} \int d\boldsymbol{x}\, c_{\theta,\theta}(\boldsymbol{x},\omega)_{kl}$$

$$c_{\theta,\theta}(\boldsymbol{x},\omega)_{kl} = \left[\mathbb{A}^{\phi}(\boldsymbol{x})^{-1}\right]_{kl} R^{\theta}_{\phi_k(\boldsymbol{x})}(\omega) R^{\theta}_{\phi_l(\boldsymbol{x})}(\omega)^{*}$$

Thank you!

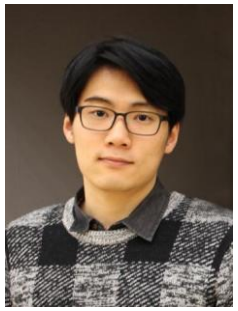
- In collaboration with…



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