量子状態統計における揺らぎの定理

辻直人

理研CEMS

Outline

Out-of-time-order fluctuation-dissipation theorem

near equilibrium

fluctuation theorem for quantum-state statistics

Tsuji, Shitara, Ueda,
Phys. Rev. E 97, 012101 (2018)

Tsuji, Ueda, arXiv:1807.11683

higher-order extension

fluctuation-dissipation theorem

near equilibrium

fluctuation theorem

Fluctuation-dissipation theorem

- Classical example: Einstein relation for Brownian motion

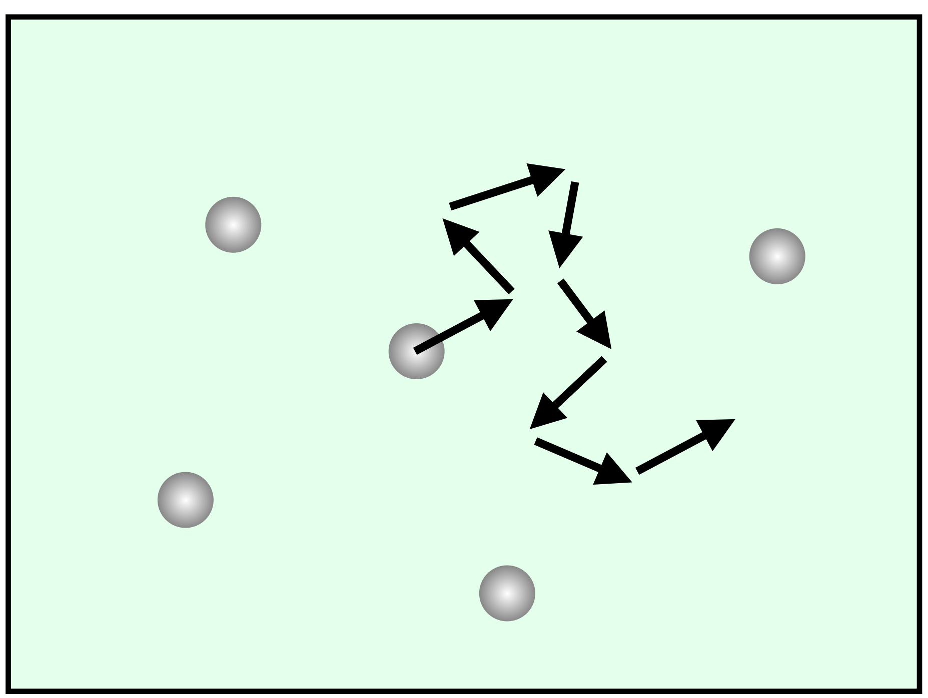
$$D = \mu k_B T$$

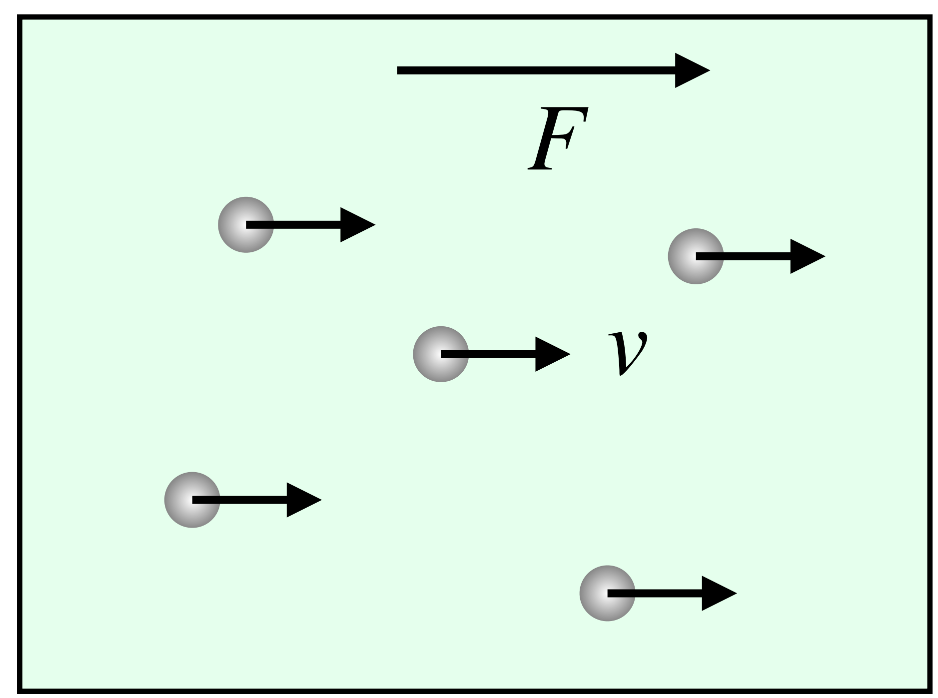
Einstein (1905)

diffusion constant

mobility $\mu = v/F$

fluctuation in equilibrium $\longleftrightarrow$ transport (dissipation) in nonequilibrium





Fluctuation-dissipation theorem

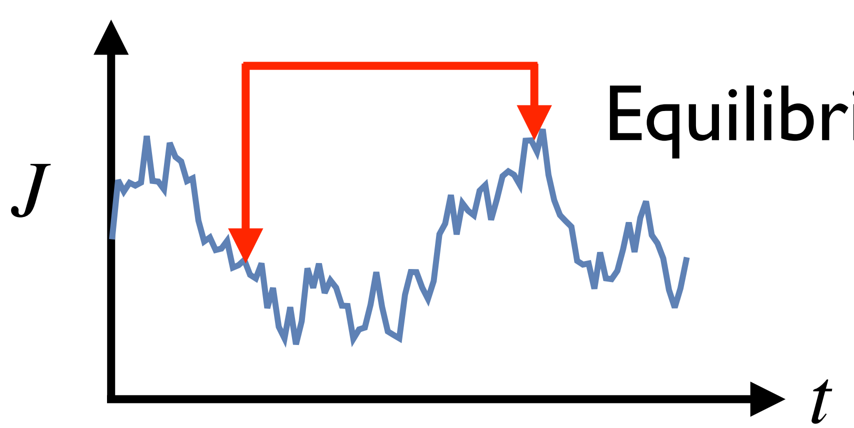
$$C_{\{A,B\}}(\omega) = \coth\left(\frac{\hbar\omega}{2k_BT}\right) C_{[A,B]}(\omega)$$

Kubo (1957)

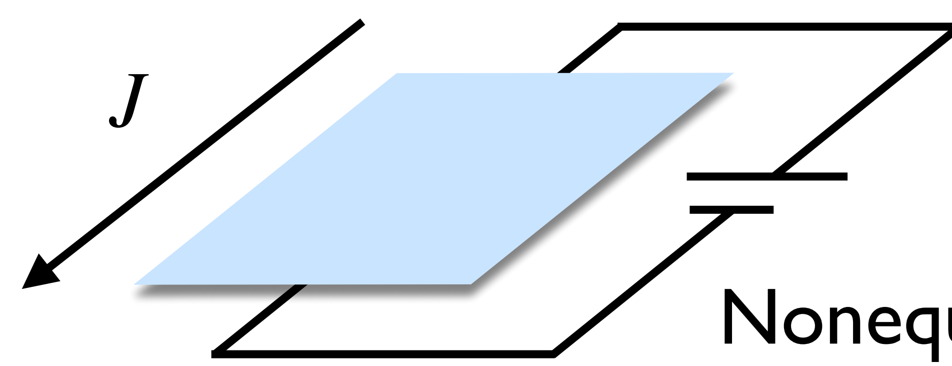
$$C_{\{A,B\}}(\omega) \equiv \int_{-\infty}^{\infty} dt e^{i\omega t}\langle\{\hat{A}(t), \hat{B}(0)\}\rangle \qquad C_{[A,B]}(\omega) \equiv \int_{-\infty}^{\infty} dt e^{i\omega t}\langle[\hat{A}(t), \hat{B}(0)]\rangle$$

fluctuation $\longleftrightarrow$ dissipation

Ex) $$\frac{V}{k_BT}\int_0^{\infty} dt\langle J_x(t)J_x(0)\rangle = \mathrm{Re}\,\sigma_{xx}(0)$$ (Green-Kubo formula)



Equilibrium



Nonequilibrium

Beyond linear response theory

- Is there any law that governs fluctuations beyond linear response theory?

- Fluctuation theorem Evans, Cohen, Morriss (1993), …

$$\frac{p(\sigma)}{\bar{p}(-\sigma)} = e^{\sigma}$$

σ : entropy production over some time interval

- Jarzynski equality Jarzynski (1997)

$$\langle e^{-\sigma} \rangle = 1 \longrightarrow \langle \sigma \rangle \geq 0$$

: 2nd law of thermodynamics

- If one applies the fluctuation theorem or Jarzysnki equality to near-equilibrium, one obtains FDT.

Beyond linear response theory

- We pursue a different direction of generalization of FDT.

- Let us consider the second moments of fluctuation and dissipation.

$$\langle\{A(t),B(0)\}^2\rangle = \underbrace{\langle A(t)B(0)A(t)B(0)\rangle}_{\text{Out-of-time-ordered correlator (OTOC)}} + \cdots$$

$$\Updownarrow ?$$

$$\langle[A(t),B(0)]^2\rangle$$

[Conventional FDT: $C_{\{A,B\}}(\omega) = \coth\left(\frac{\hbar\omega}{2k_BT}\right) C_{[A,B]}(\omega)$]

Question: Is there any relation among them?

Out-of-time-order FDT

Tsuji, Shitara, Ueda, Phys. Rev. E 97, 012101 (2018)

$$C_{\{A,B\}^2}(\omega) + C_{[A,B]^2}(\omega) = 2\coth\left(\frac{\hbar\omega}{4k_B T}\right) C_{\{A,B\}[A,B]}(\omega)$$

OTOC w/ bipartite statistical average:

Maldacena, Shenker, Stanford (2015), …

$$C_{\{A,B\}^2}(t,t') \equiv \mathrm{Tr}(\hat{\rho}^{\frac{1}{2}}\{\hat{A}(t),\hat{B}(t')\}\hat{\rho}^{\frac{1}{2}}\{\hat{A}(t),\hat{B}(t')\})$$

cf. OTOC w/ usual statistical average:

$$\tilde{C}_{\{A,B\}^2}(t,t') \equiv \mathrm{Tr}(\hat{\rho}\{\hat{A}(t),\hat{B}(t')\}\{\hat{A}(t),\hat{B}(t')\})$$

$$\hat{\rho} = e^{-\beta H}/Z$$

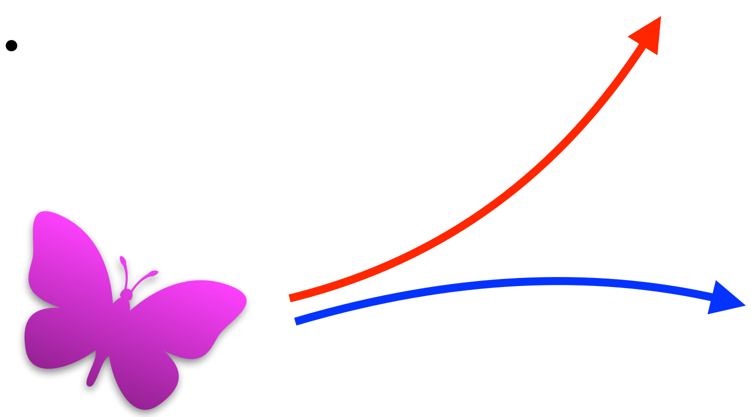
Physical interpretation

Tsuji, Shitara, Ueda, Phys. Rev. E 97, 012101 (2018)

$$C_{\{A,B\}^2}(\omega) + C_{[A,B]^2}(\omega) = 2\coth\left(\frac{\hbar\omega}{4k_B T}\right) C_{\{A,B\}[A,B]}(\omega)$$

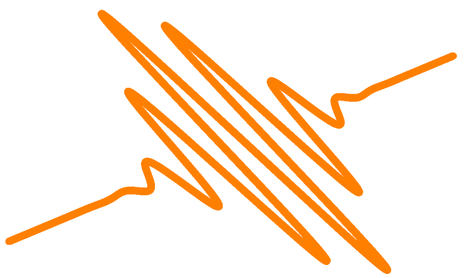
- (LHS): butterfly effect (chaotic properties).

$$C_{\{A,B\}^2}(t,0) + C_{[A,B]^2}(t,0) \sim e^{\lambda t}$$

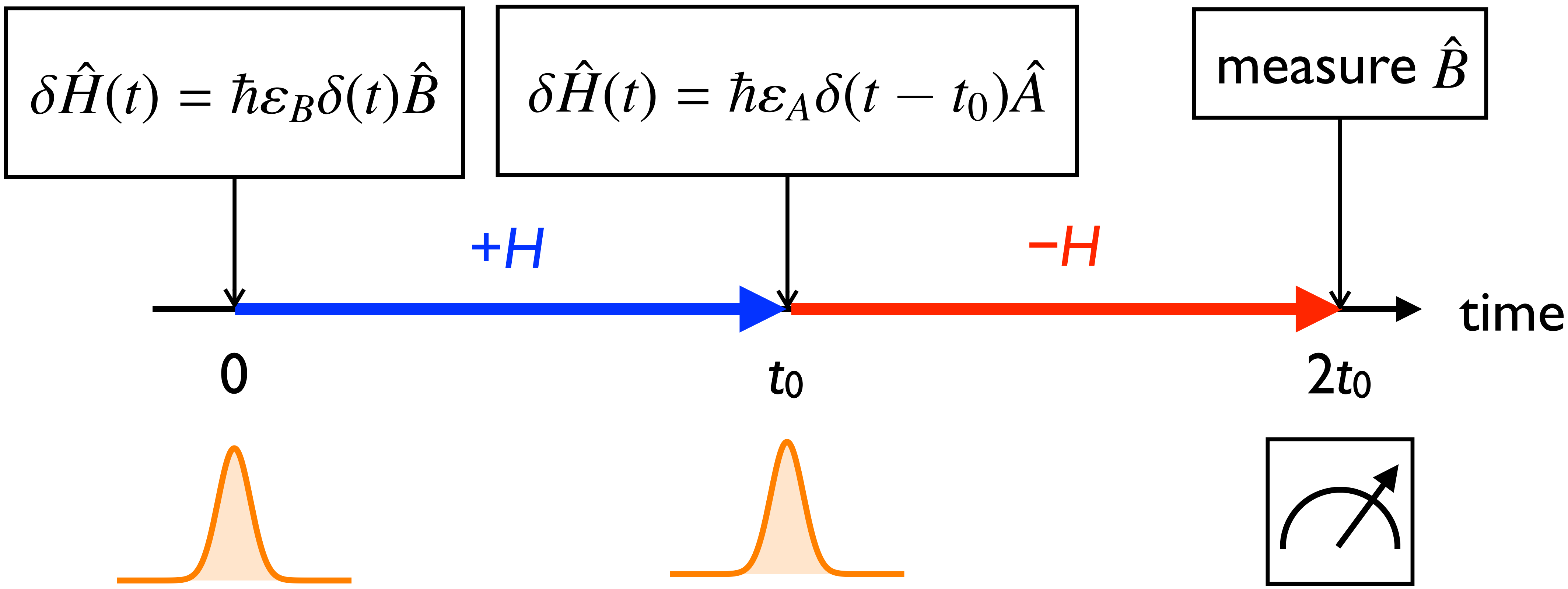


- (RHS): certain nonlinear response function

$$2C_{\{A,B\}[A,B]}(t,0) \sim i[L^{(3)}_{(AB)^2}(t) + L^{(1)}_{A^2B^2}(t)]$$



Nonlinear response function



$$\langle \hat{B}(2t_0)\rangle = \sum_{m,n=0}^{\infty} \varepsilon_A^m \varepsilon_B^n [\delta^{m+n}_{A^m B^n} \langle \hat{B}(2t_0)\rangle] \qquad \delta^3_{A^2 B}\langle \hat{B}(2t_0)\rangle =: \frac{1}{2} L^{(3)}_{(AB)^2}(t_0, 0)$$

- The usual perturbation theory gives

$$2C_{\{A,B\}[A,B]}(t,0) \sim i[L^{(3)}_{(AB)^2}(t) + L^{(1)}_{A^2B^2}(t)]$$

Up to the difference of usual and bipartite statistical averages

Difference of statistical averages

- Bipartite statistical average:

$$C_{\{A,B\}^2}(t,t') \equiv \mathrm{Tr}(\hat{\rho}^{\frac{1}{2}}\{\hat{A}(t),\hat{B}(t')\}\hat{\rho}^{\frac{1}{2}}\{\hat{A}(t),\hat{B}(t')\})$$

$\rightarrow$ OTO-FDT

- Usual statistical average:

$$\tilde{C}_{\{A,B\}^2}(t,t') \equiv \mathrm{Tr}(\hat{\rho}\{\hat{A}(t),\hat{B}(t')\}\{\hat{A}(t),\hat{B}(t')\})$$

- The difference is represented by Wigner-Yanase skew information.

Tsuji, Shitara, Ueda, Phys. Rev. E 97, 012101 (2018)

Wigner-Yanase skew information:

$$I_{\frac{1}{2}}(\hat{\rho},\hat{O}) \equiv -\frac{1}{2}\mathrm{Tr}([\hat{\rho}^{\frac{1}{2}},\hat{O}]^2)$$ Wigner, Yanase (1963)

$$= \mathrm{Tr}(\hat{\rho}\hat{O}^2) - \mathrm{Tr}(\hat{\rho}^{\frac{1}{2}}\hat{O}\hat{\rho}^{\frac{1}{2}}\hat{O})$$

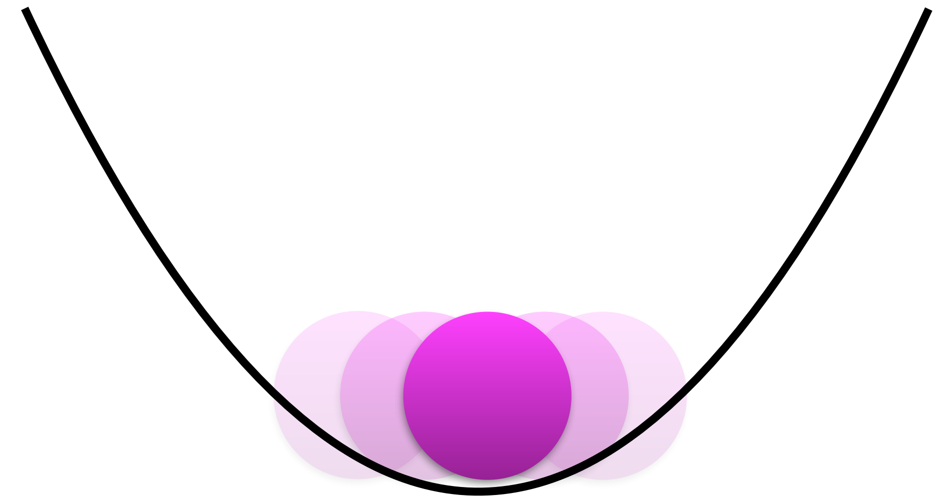
Skew information

- Wigner-Yanase skew information quantifies information contents of "quantum fluctuation" of O for a state ρ.

$$\underbrace{\langle(\Delta\hat{O})^2\rangle}_{\text{variance}} = \underbrace{C(\hat{\rho},\hat{O})}_{\text{classical}} + \underbrace{Q(\hat{\rho},\hat{O})}_{\text{quantum}}$$

$$\text{quantum} = I_{\frac{1}{2}}(\hat{\rho},\hat{O})$$

$$\Delta\hat{O} \equiv \hat{O} - \langle\hat{O}\rangle$$



- OTO-FDT w/ usual statistical average:

$$\tilde{C}_{\{A,B\}^2}(\omega) + \tilde{C}_{[A,B]^2}(\omega)$$
$$= \coth\left(\frac{\hbar\omega}{4k_BT}\right)[\tilde{C}_{\{A,B\}[A,B]}(\omega) + \tilde{C}_{[A,B]\{A,B\}}(\omega)] + \underbrace{I_{AB}(\omega)}_{\text{skew information}}$$

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near equilibrium ←

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↑ higher-order extension

fluctuation-dissipation theorem

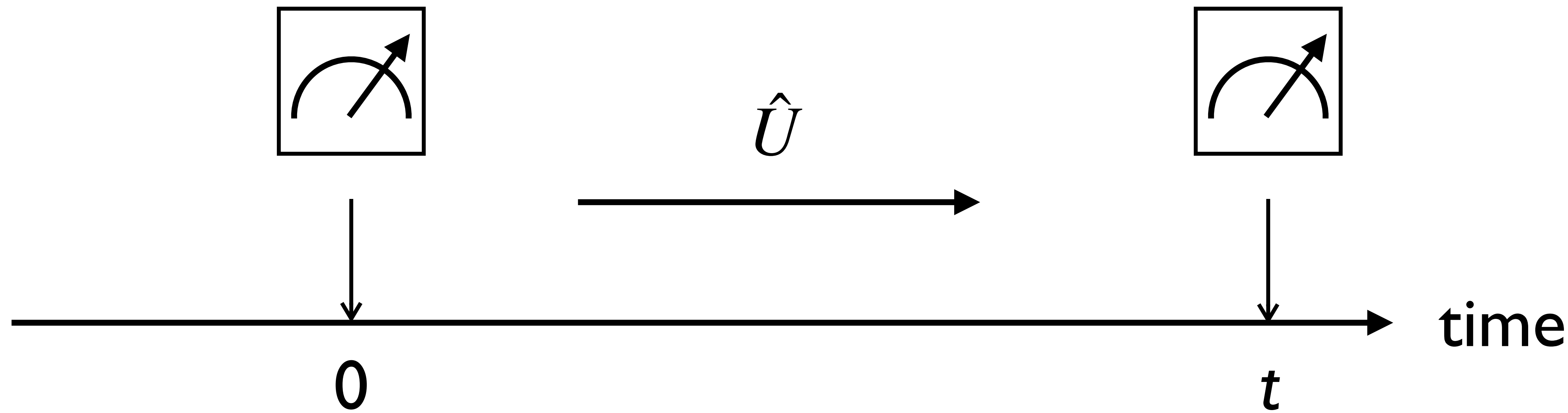
near equilibrium ←

fluctuation theorem

Quantum work FT

Kurchan (2000), Tasaki (2000)

- Two-point measurement for the work



$$\hat{\rho}_i = \frac{e^{-\beta \hat{H}}}{Z} \longrightarrow \hat{\rho}(E_k^i) \longrightarrow \hat{\rho}^U = \hat{U}\hat{\rho}(E_k^i)\hat{U}^\dagger$$

$$= |E_k^i\rangle\langle E_k^i|$$

work: $\quad w = E_l^f - E_k^i$

probability: $\quad p = \langle E_k^i|\hat{\rho}_i|E_k^i\rangle\langle E_l^f|\hat{\rho}^U|E_l^f\rangle$

Quantum work FT

Kurchan (2000), Tasaki (2000)

- Work probability distribution

$$p(w) = \sum_{kl} \delta(w - E_l^f + E_k^i) \langle E_k^i | \hat{\rho}_i | E_k^i \rangle \langle E_l^f | \hat{\rho}^U | E_l^f \rangle$$

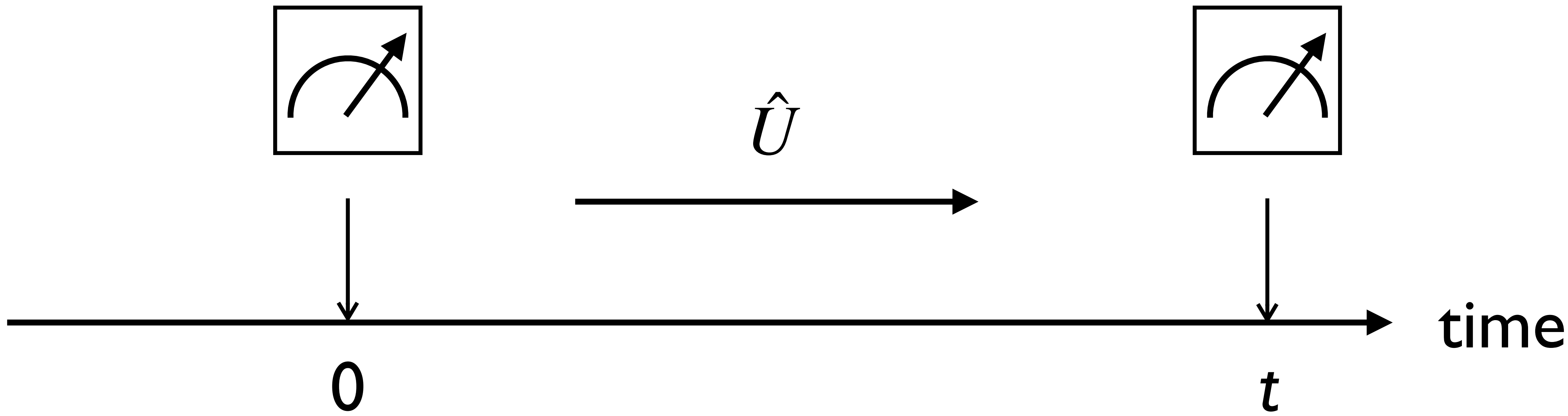
- Fluctuation theorem (Crooks relation)

$$\frac{p(w)}{\bar{p}(-w)} = e^{\beta(w - \Delta F)}$$

$\Delta F = F_f - F_i$: equilibrium free-energy difference

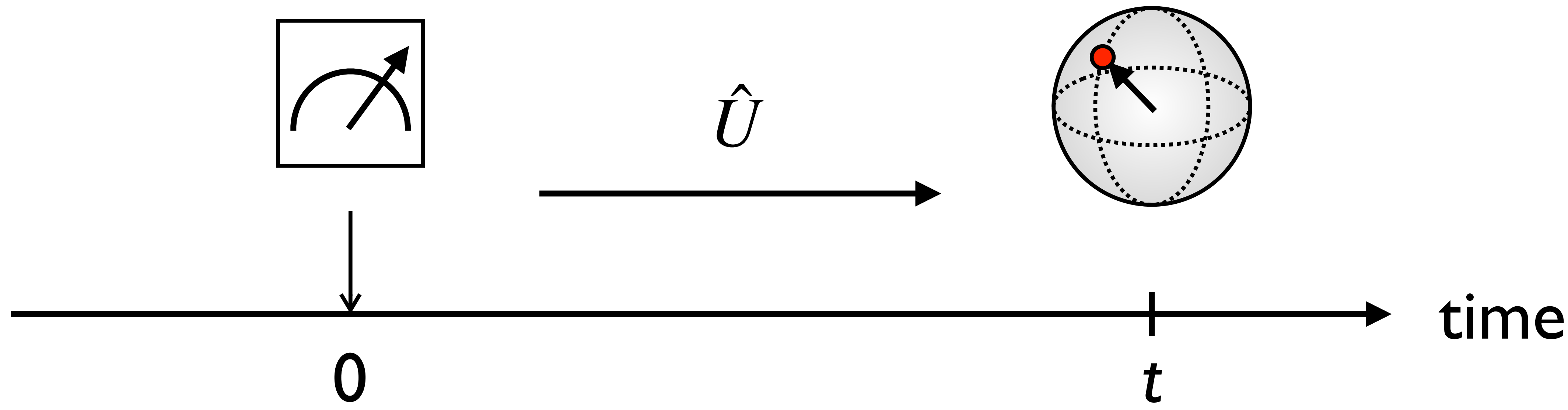
- Jarzynski relation

$$\langle e^{-\beta w} \rangle = e^{-\beta \Delta F} \longrightarrow \langle w \rangle \geq \Delta F$$: second law



$$\hat{\rho}_i \longrightarrow \hat{\rho}(E_k^i) = |E_k^i\rangle\langle E_k^i| \longrightarrow \hat{\rho}^U = \hat{U}\hat{\rho}(E_k^i)\hat{U}^\dagger$$

- In the above scheme, one obtains limited information on the quantum state $\hat{\rho}^U$, i.e., only the diagonal component $\langle E_l^f|\hat{\rho}^U|E_l^f\rangle$ is available.



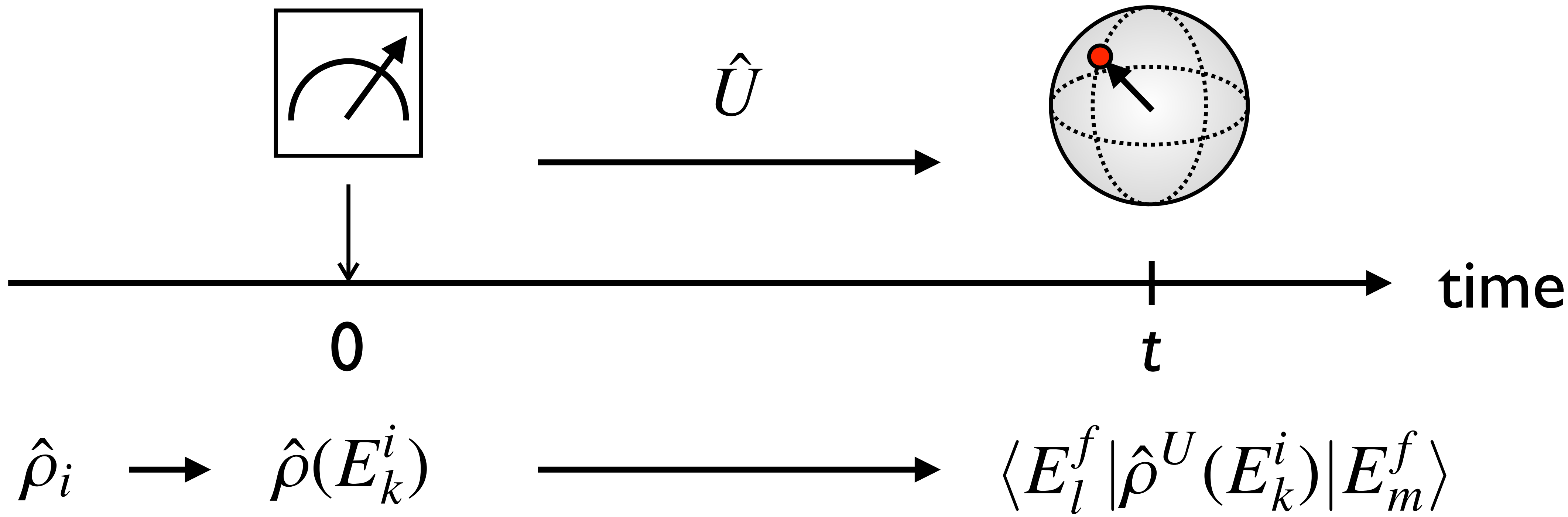
$$\hat{\rho}_i \longrightarrow \hat{\rho}(E_1^i) \longrightarrow \langle E_l^f|\hat{\rho}^U(E_1^i)|E_m^f\rangle$$

$$\hat{\rho}_i \longrightarrow \hat{\rho}(E_2^i) \longrightarrow \langle E_l^f|\hat{\rho}^U(E_2^i)|E_m^f\rangle$$

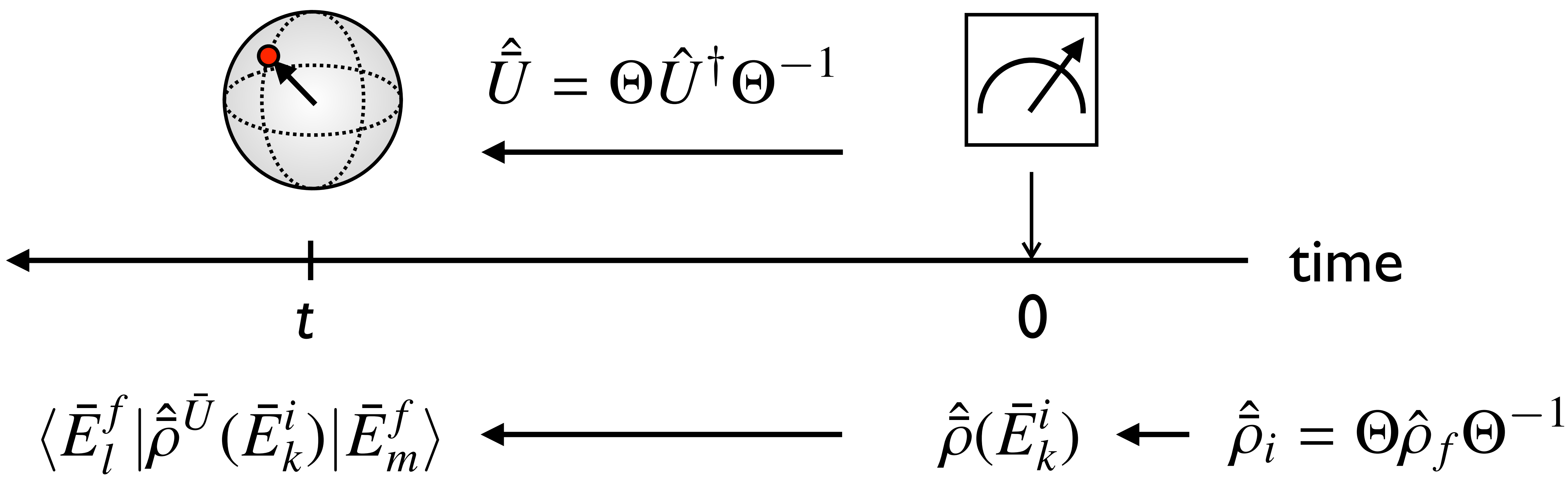
$$\vdots \qquad\qquad \vdots$$

Question: How does the quantum state, including off-diagonal components $\langle E_l^f|\hat{\rho}^U|E_m^f\rangle$, distribute?

- Forward process



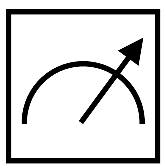
- Backward process



Quantum state statistics

Tsuji, Ueda, arXiv:1807.11683

energy measurement



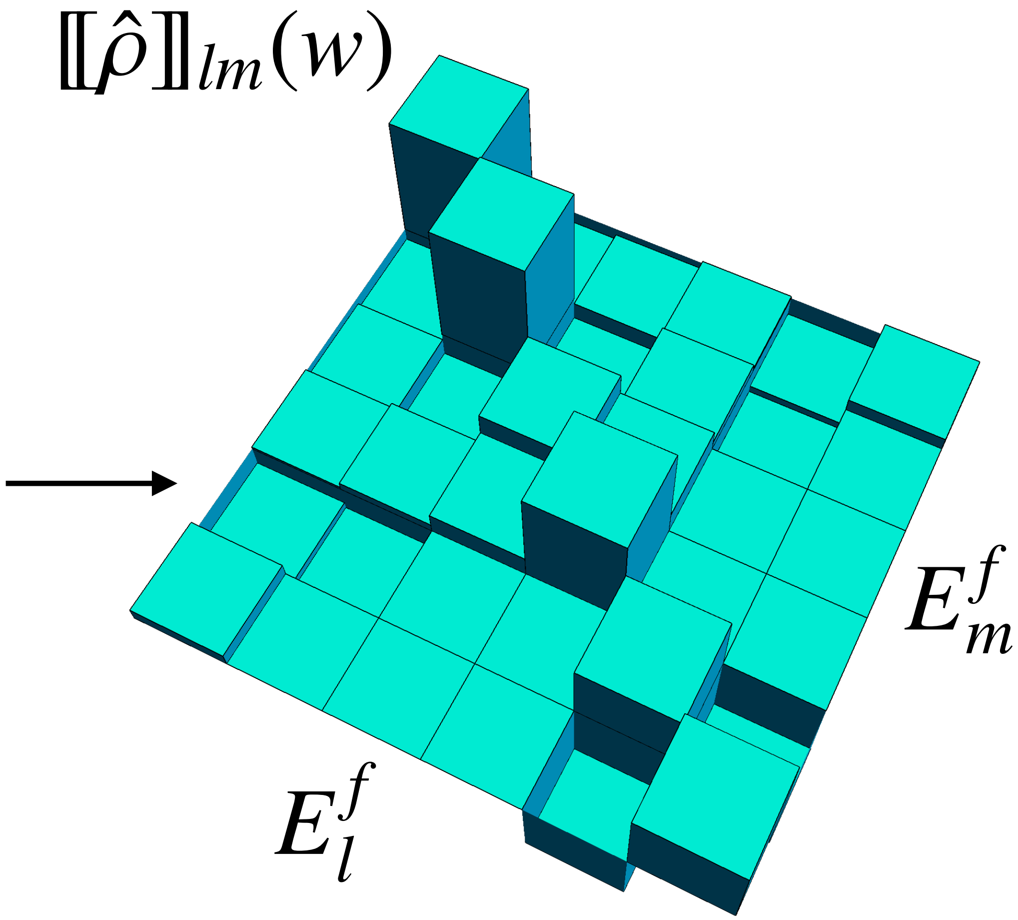
$$\hat{\rho}_i \longrightarrow \hat{\rho}(E_1^i) \xrightarrow{\hat{U}} \langle E_l^f|\hat{\rho}^U(E_1^i)|E_m^f\rangle$$

$$\hat{\rho}_i \longrightarrow \hat{\rho}(E_2^i) \longrightarrow \langle E_l^f|\hat{\rho}^U(E_2^i)|E_m^f\rangle$$

$$\vdots \qquad\qquad \vdots$$

quantum-state data

$\longrightarrow$



$$[\![\hat{\rho}]\!]_{lm}(w) = \overline{\delta(w - (\tfrac{1}{2}(E_l^f + E_m^f) - E_k^i))\langle E_l^f|\hat{\rho}^U(E_k^i)|E_m^f\rangle}$$

Quantum state statistics

- Distribution function defined by the *n*-th moment

$$p_n(w) \equiv \frac{1}{\mathcal{N}_n} \mathrm{Tr}([\![\hat{\rho}]\!]^{\circledast n}(w)) \quad (n = 1, 2, \ldots)$$

$$([\![\hat{\rho}]\!] \circledast [\![\hat{\rho}]\!])_{lm}(w) \equiv \int_{-\infty}^{\infty} dw' \sum_n [\![\hat{\rho}]\!]_{ln}(w - w')[\![\hat{\rho}]\!]_{nm}(w')$$

$$\int_{-\infty}^{\infty} dw\, p_n(w) = 1 \qquad\qquad p_n(w) \in \mathbb{R}$$

- $p_1(w)$ is the work probability distribution.
- $p_n(w) \;\; (n \geq 2)$ is not necessarily positive semidefinite.

→ quasiprobability distribution

FT for quantum state statistics

Tsuji, Ueda, arXiv:1807.11683

$$\frac{p_n(w)}{\bar{p}_n(-w)} = e^{\beta(w - n\Delta F(n\beta))} \quad (n = 1, 2, \ldots)$$

- For n=1, the relation reduces to the quantum work FT.

- For n>=2, the relation gives an extension of the quantum work FT to quantum state statistics.

- (LHS): $p_n(w)$ and $\bar{p}_n(-w)$ strongly depends on $\hat{U}$.

- (RHS): only depends on the equilibrium quantities.

Integral FT for quantum state statistics

Tsuji, Ueda, arXiv:1807.11683

$$\langle e^{-\beta w} \rangle_{p_n} = e^{-n\beta \Delta F(n\beta)} \quad (n = 1, 2, \dots)$$

- For n=1, the relation reduces to the Jarzynski equality.
- One might be tempted to derive an inequality,

$$\langle w \rangle_{p_n} \geq n\Delta F(n\beta) \quad (!)$$

- This is, however, possible only if $p_n(w)$ is positive semidefinite.
- $p_n(w)$ $(n \geq 2)$ is not necessarily positive semidefinite.

Characteristic function

$$G_n(u) \equiv \int_{-\infty}^{\infty} dw\, e^{iuw} p_n(w) \quad (n = 1, 2, \dots)$$

- $G_n(u) \ (n \geq 2)$ is an out-of-time-ordered correlation function.

$$G_2(u) = \frac{1}{\mathcal{N}_2} \mathrm{Tr}[\hat{\rho}_i \hat{W}^\dagger_{i,u}(0) \hat{W}_{f,u}(t) \hat{\rho}_i \hat{W}^\dagger_{i,u}(0) \hat{W}_{f,u}(t)]$$

$$\hat{W}_{i,u} = e^{iu\hat{H}_i} \qquad \hat{W}_{f,u} = e^{iu\hat{H}_f}$$

- $G_n(u)$ satisfies a symmetry relation,

$$G_n(u) = \frac{Z_f(n\beta)}{Z_i(n\beta)} \bar{G}_n(-u + i\beta) \quad \rightarrow \quad \frac{p_n(w)}{\bar{p}_n(-w)} = e^{\beta(w - n\Delta F(n\beta))}$$

Derivation of OTO-FDT

- Cumulant expansion of the integral FT up to third order.

$$\langle w \rangle_{p_1}|_{\beta} - \Delta F(\beta) \approx \frac{\beta}{2}\langle (\Delta w)^2 \rangle_{p_1}|_{\beta} - \frac{\beta^2}{6}\langle (\Delta w)^3 \rangle_{p_1}|_{\beta}$$

$$\frac{1}{2}\langle w \rangle_{p_2}|_{\frac{\beta}{2}} - \Delta F(\beta) \approx \frac{\beta}{8}\langle (\Delta w)^2 \rangle_{p_2}|_{\frac{\beta}{2}} - \frac{\beta^2}{48}\langle (\Delta w)^3 \rangle_{p_2}|_{\frac{\beta}{2}}$$

- Perturbative expansion up to the second order around the equilibrium.

$$C_{\{A,B\}[A,B]}(\omega) \approx \frac{\beta\hbar\omega}{8}[C_{\{A,B\}^2}(\omega) + C_{[A,B]^2}(\omega)]$$

→ near-zero-frequency part of OTO-FDT

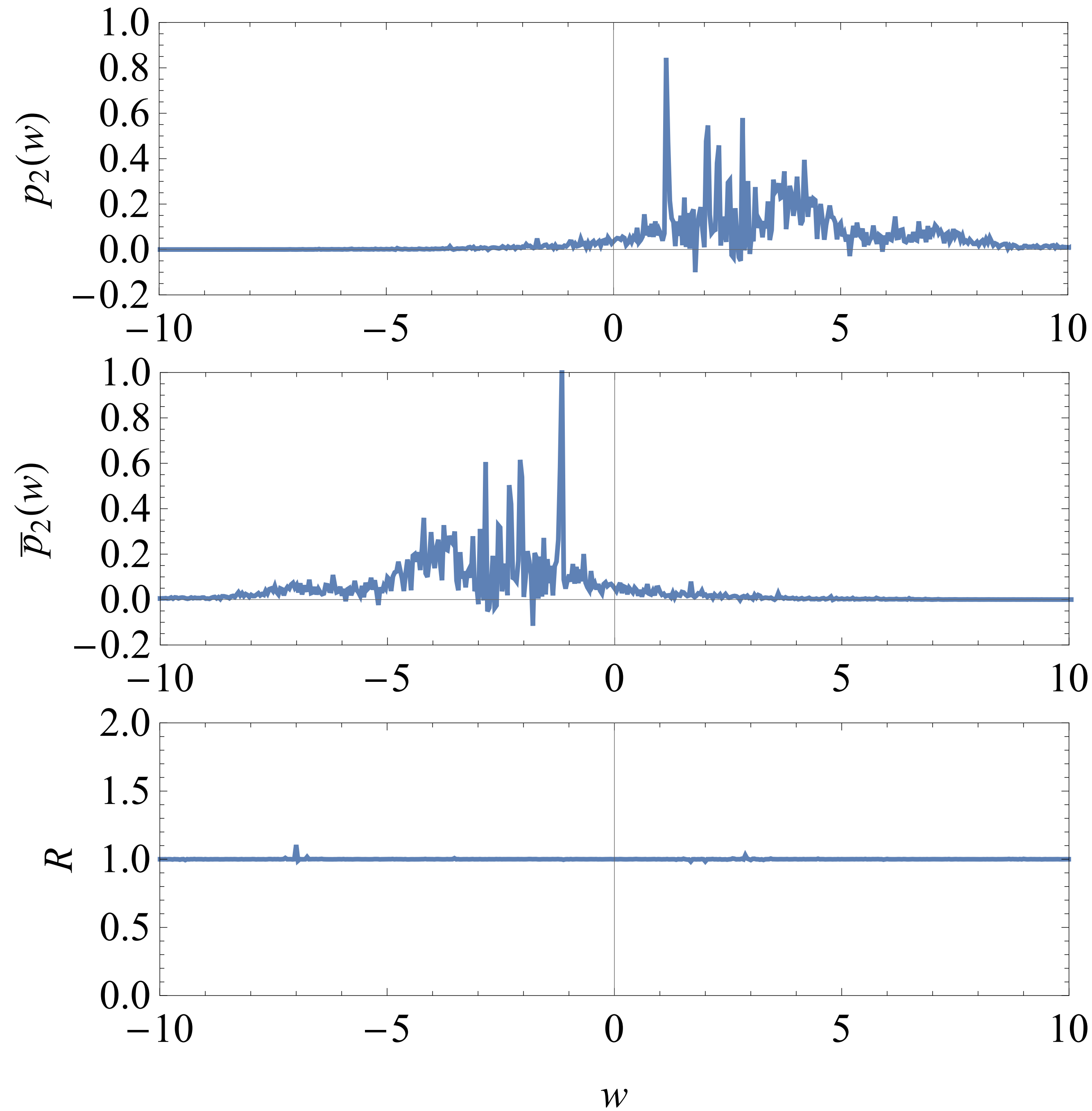
Numerical test of QSS FT

- 1D hardcore boson model

$$\hat{H}(s) = -t\sum_i (b_i^\dagger b_{i+1} + \text{h.c.}) + V(s)\sum_i n_i^b n_{i+1}^b - t'\sum_i (b_i^\dagger b_{i+2} + \text{h.c.}) + V'\sum_i n_i^b n_{i+2}^b$$

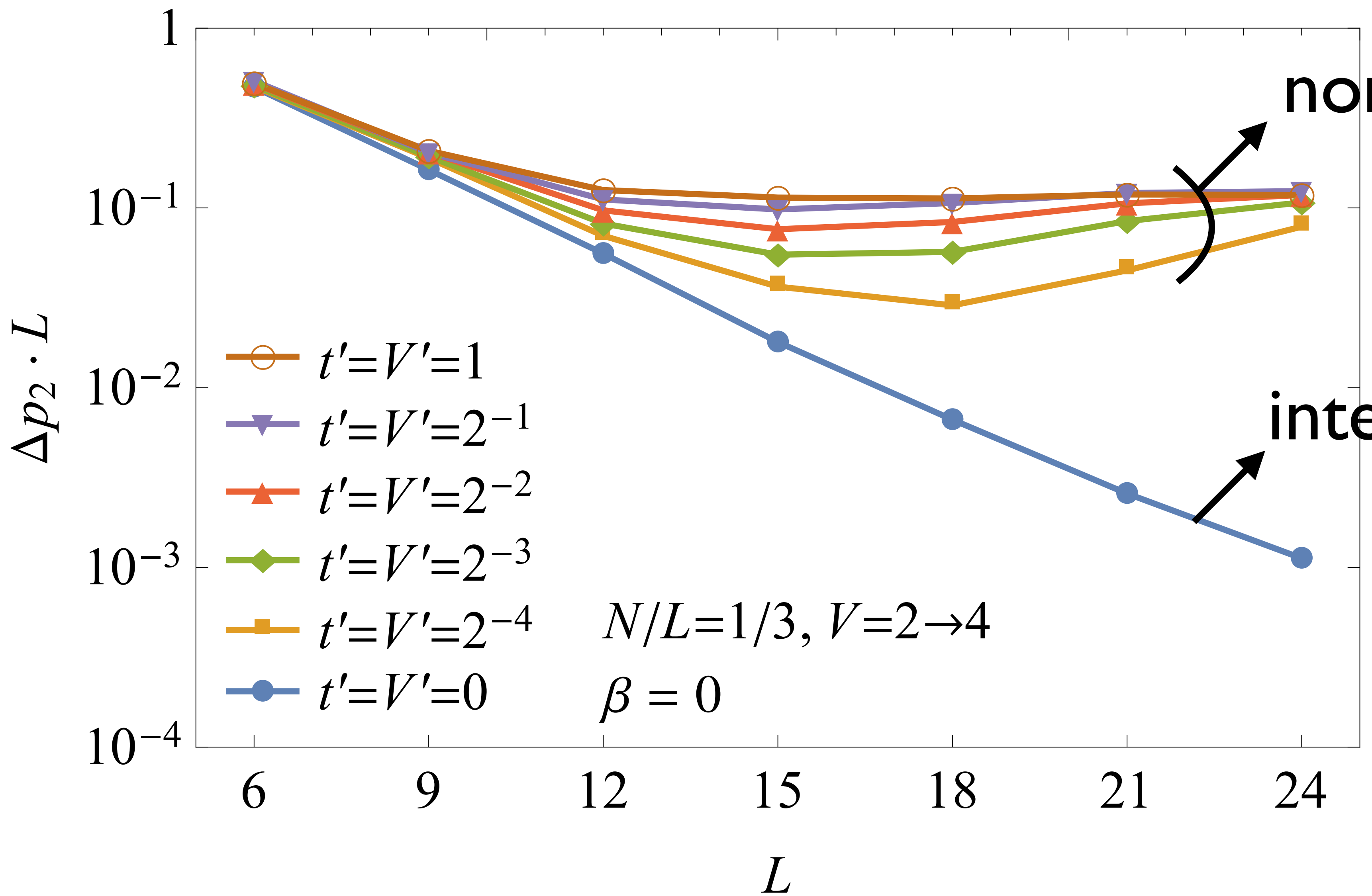
$$V = 2 \to 4, t' = V' = 1,$$
$$\beta = 0.1, L = 12, N = 4$$
$$\Delta w = 0.04$$

$$R = p_2(w)/\bar{p}_2(-w)/e^{\beta(w-2\Delta F(2\beta))}$$



Fluctuation of QSS

$$\Delta p_2 \equiv \frac{1}{Z_i(\beta)}\|p_2\|_1 = \frac{1}{Z_i(\beta)}\int_{-\infty}^{\infty} dw\,|p_2(w)| \qquad \Delta p_2 \leq \frac{\sum_\alpha D_\alpha^2}{(\sum_\alpha D_\alpha)^2}$$



non-integrable

$\Delta p_2 \sim L^{-1}$

integrable

$\Delta p_2 \sim e^{-cL}$

Summary

- We proved the fluctuation theorem for quantum state statistics.

Tsuji, Ueda, arXiv:1807.11683

$$\frac{p_n(w)}{\bar{p}_n(-w)} = e^{\beta(w - n\Delta F(n\beta))} \quad (n = 1, 2, \ldots)$$

- n=1 corresponds to the quantum work FT.
- n=2 reproduces OTO-FDT near equilibrium.
- Fluctuation of quantum state statistics <=> quantum chaos
- And what else ? …