imagine the impossible

KIAS KOREA INSTITUTE FOR ADVANCED STUDY

Microscopic reversibility in the quantum regime

Nonequilibrium Statistical Physics of Complex Systems
The 10th Conference on Statistical Physics
2024. 07. 25. @KIAS

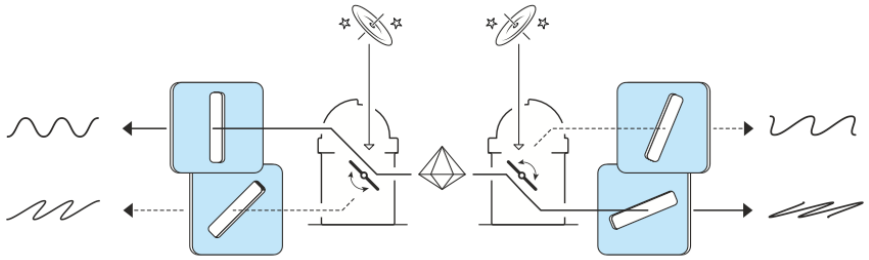
Hyukjoon Kwon
School of Computational Sciences
Korea Institute for Advanced Study

[M. Bellini, HK, N. Biagi, S. Francesconi, A. Zavatta, and M. S. Kim, PRL 129, 170604]

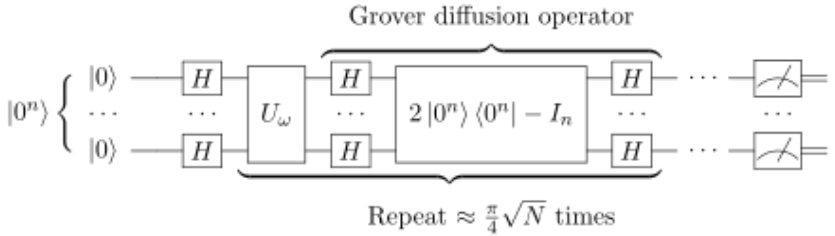
Theory with M. S. Kim (Imperial College London)
Experimental collaboration with Marco Bellini's group at CNR-INO (Univ. Firenze)

As a physicist working on quantum information theory…

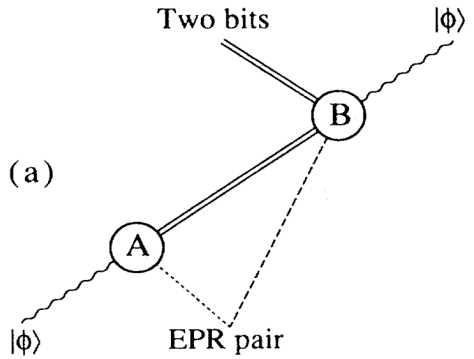
- **What I usually talk about in a conference**



Quantum entanglement,
(Bell nonlocality)



Quantum computing, algorithm, complexity



Quantum teleportation
(communication)



- **But I also do care about thermodynamics/non-equilibrium physics**

As a physicist working on quantum information theory…

- **But I also do care about thermodynamics/non-equilibrium physics**

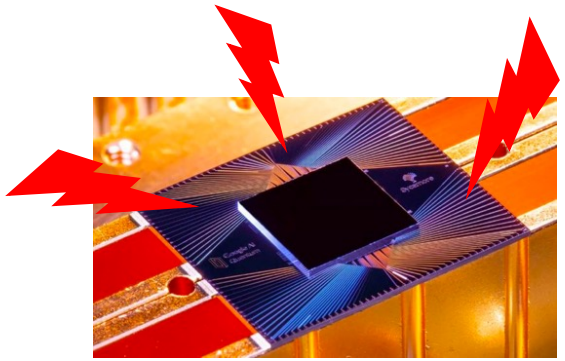
Why?

For a better understanding of our nature
- Extending thermodynamics laws
  (e.g., von Neumann "entropy")

$$S(\rho) = -\mathrm{Tr}[\rho \log \rho]$$

- Understand the role of quantum resources
  (coherence/entanglement)

Quantum noise ⇔ non-equilibrium dynamics



- Characterizing & overcoming quantum noise

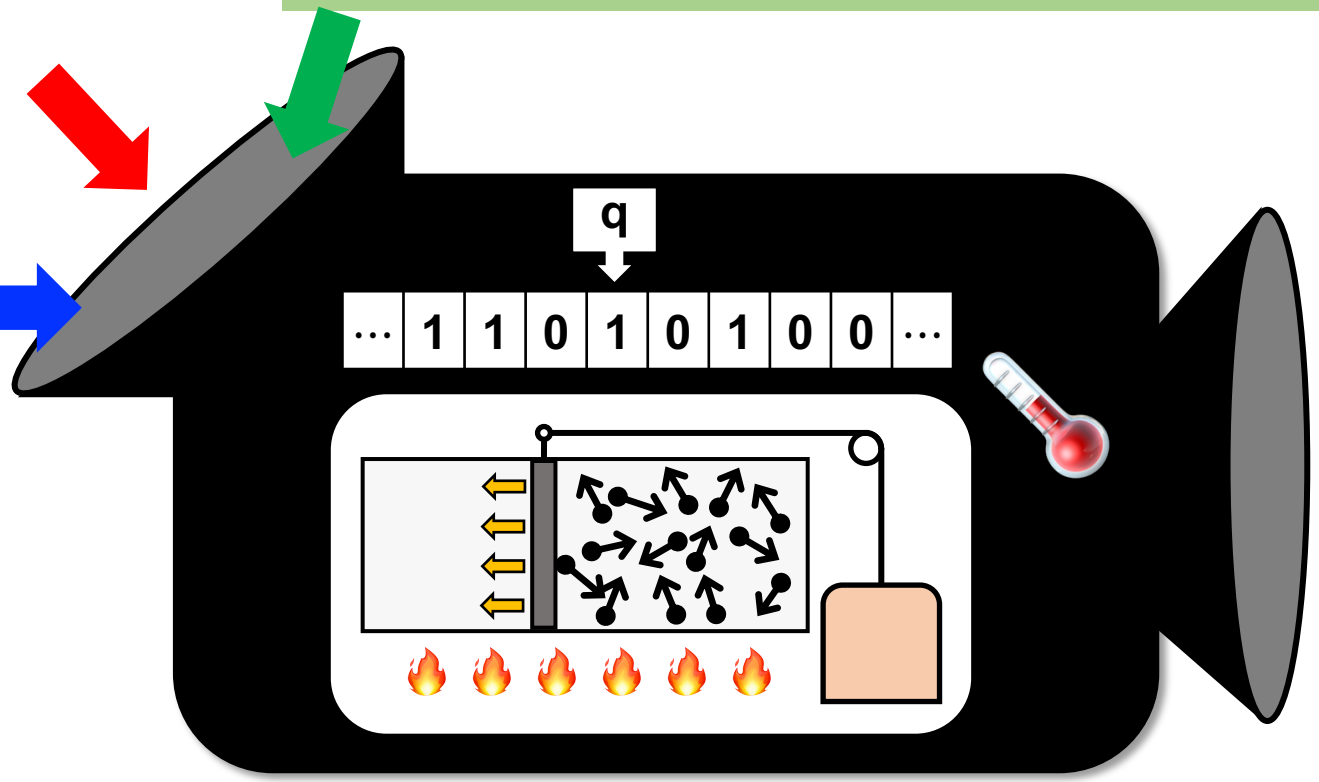
We can learn from each other
- Many interesting talks throughout this conference
- TUR (Thermodynamic uncertainty relation)
- Speed limit
  Quantum: Mandelshtam & Tamm (1945), Margolus–Levitin (1998)]
  Classical stochastic process: N. Shiraishi, K. Funo, K. Saito, PRL 121, 070601 (2018)
- We can actually work together! [J. Lee, S. Lee, HK, H. Park, PRL 129, 120603 (2022)]

Quantum information theory and thermodynamics

Energy

Information

Quantum information (coherence/entanglement)



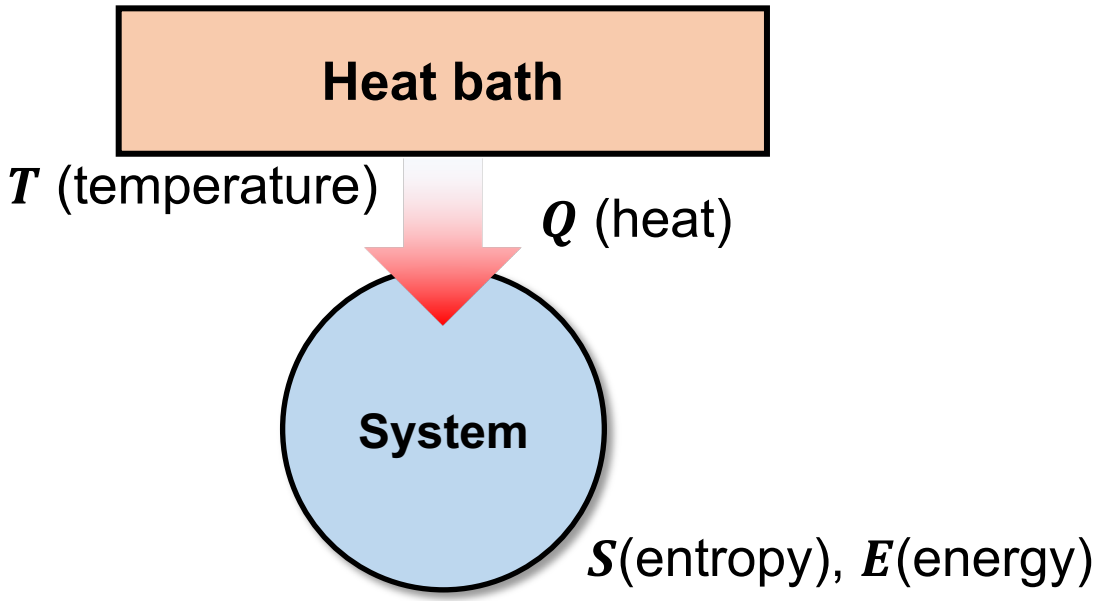
Thermodynamics process (e.g., heat engine)
+ Information processing

Landauer's principle

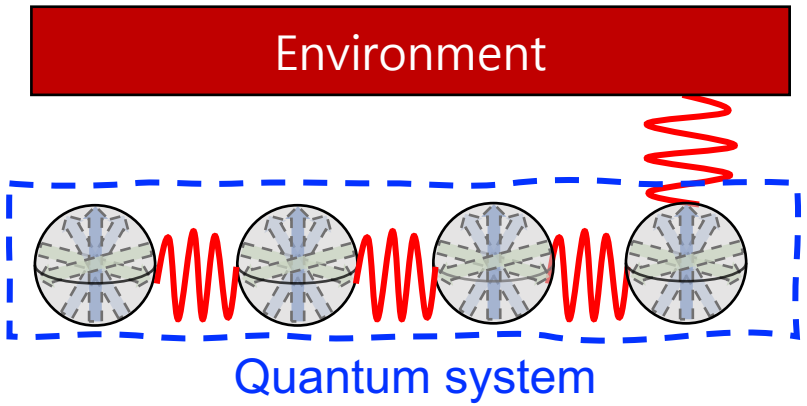
Universal physical law?

“The second law of thermodynamics”
(Macroscopic irreversibility)

Quantum vs. classical thermodynamics



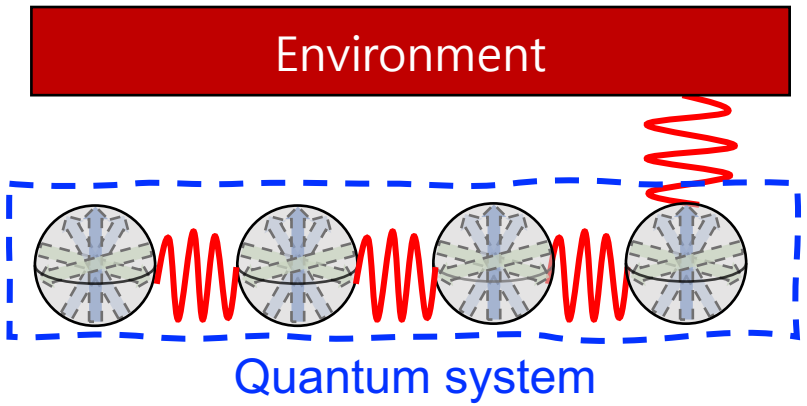
Quantum vs. classical thermodynamics



Open quantum dynamics (quantum channel):

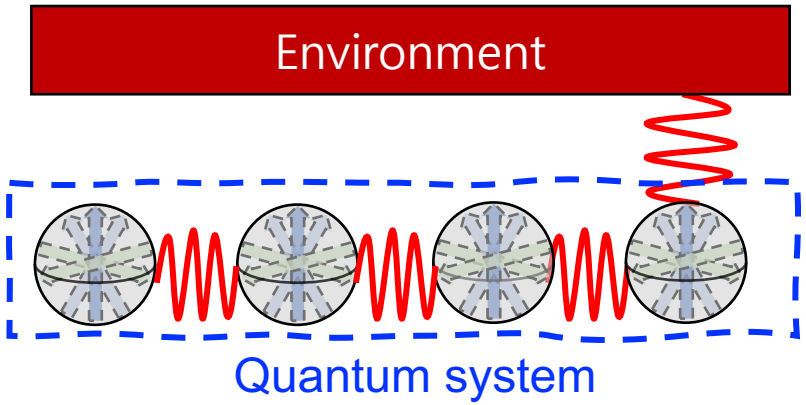
- A quantum system interacts with external environment
- The dynamics is no more unitary (thus, in general irreversible dynamics)

Quantum vs. classical thermodynamics



1. **How to define thermodynamic quantities (entropy production & heat)?**
2. **How to deal with superposition (coherence) during the process?**
3. **What is a time-reversal process?**

Quantum vs. classical thermodynamics



1. **How to define thermodynamic quantities (entropy production & heat)?**

2. **How to deal with superposition (coherence) during the process?**

3. **What is a time-reversal process?**

Recent developments (entirely from quantum information perspectives)

M. D. Vidrighin, O. Dahlsten, M. Barbieri, M. S. Kim, V. Vedral, and I. A. Walmsley, PRL **116**, 050401 (2016).
J. Åberg, PRX **8**, 011019 (2018).
G. Manzano, J. M. Horowitz, and J. M. R. Parrondo, PRX **8**, 031037 (2018).
Z. Holmes, S. Weidt, D. Jennings, J. Anders, and F. Mintert, Quantum **3**, 124 (2019).
HK and M. Kim, PRX **9**, 031029 (2019).
K. Micadei, G. T. Landi, and E. Lutz, PRL **124**, 090602 (2020).
⋮

In this talk…

- **Main question:**
  Can we find a fundamental difference between quantum & classical thermodynamic principles?

- **Checklist**

Fundamental thermodynamic principle?	
A simple classical/quantum process?	
What makes the difference?	
What is the correction?	
Classical limit?	
How to test it?	

In this talk…

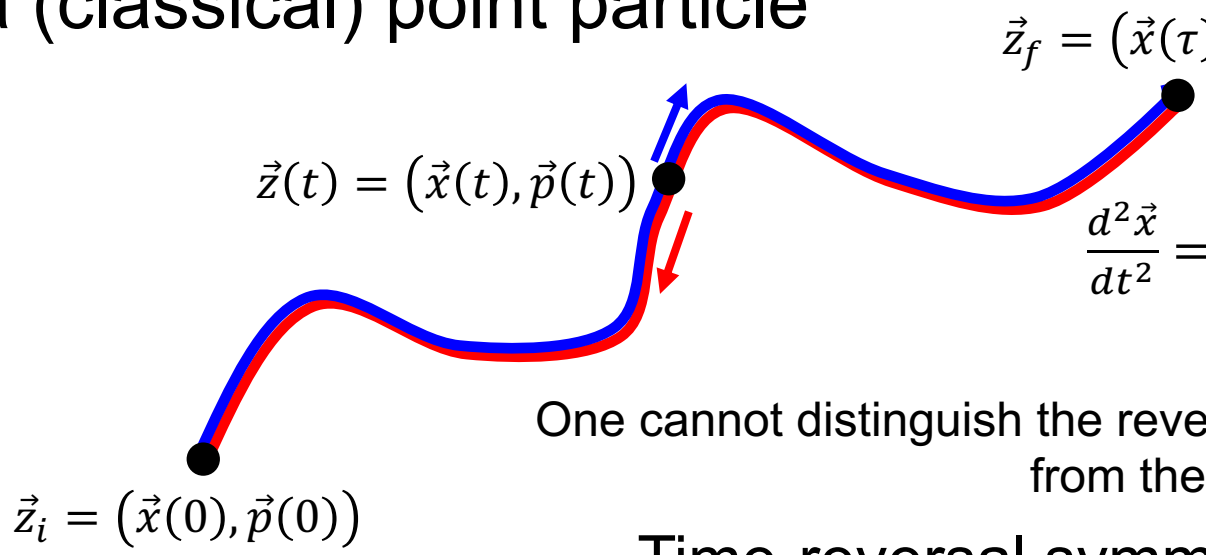
- **Main question:**
  Can we find a fundamental difference between quantum & classical thermodynamic principles?

- **Checklist**

Fundamental thermodynamic principle?	Microscopic reversibility
A simple classical/quantum process?	
What makes the difference?	
What is the correction?	
Classical limit?	
How to test it?	

Microscopic reversibility vs. Macroscopic irreversibility

- Consider a (classical) point particle

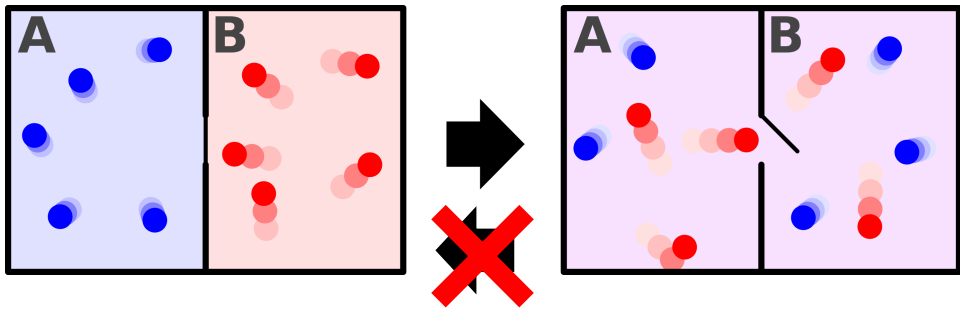


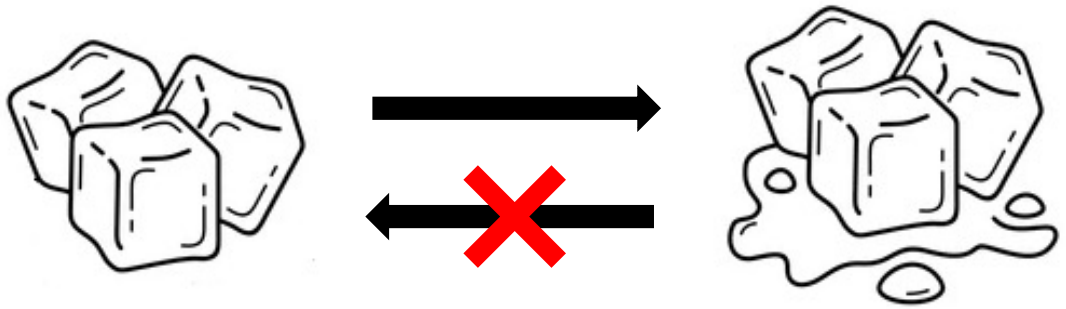
$\frac{d^2\vec{x}}{dt^2} = \frac{\vec{F}}{m}$ (Equation of motion)

One cannot distinguish the reverse trajectory $(t \to -t)$ & $(x, p) \to (x, -p)$ from the forward trajectory

Time-reversal symmetry (microscopic reversibility)

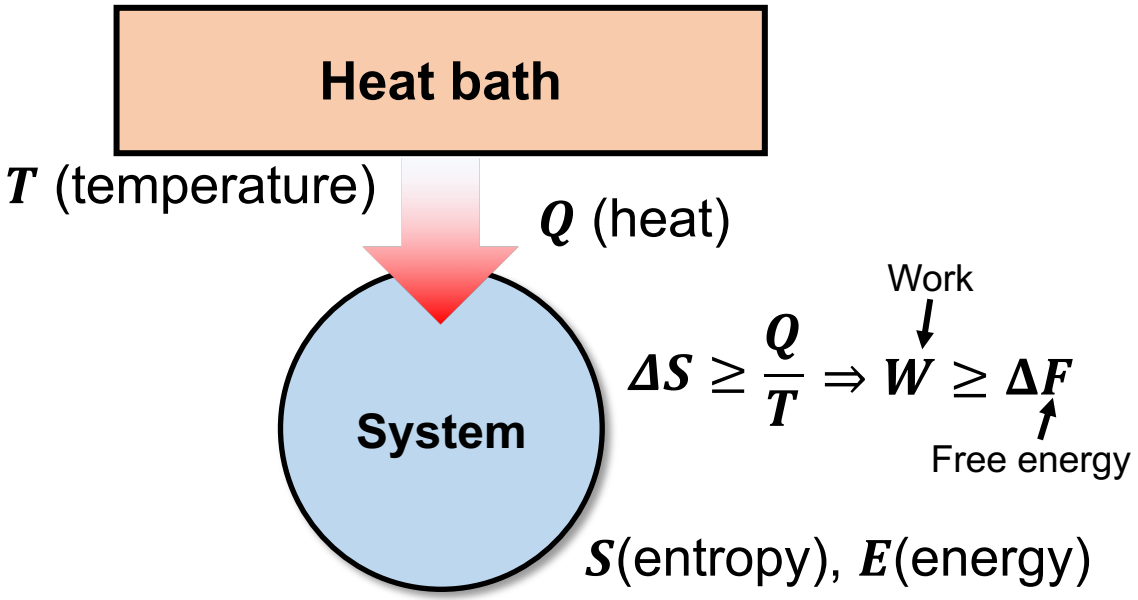
- However, for a macroscopic object





Arrow of time (Macroscopic irreversibility)

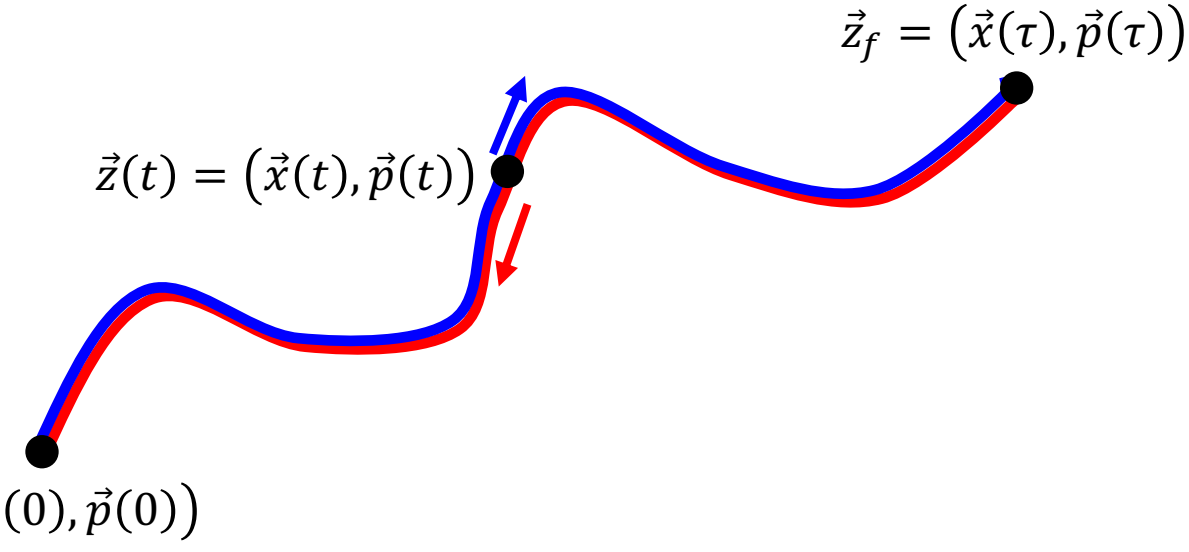
Microscopic reversibility (classical)



$$\Delta S \geq \frac{Q}{T} \Rightarrow W \geq \Delta F$$

Work

Free energy



- **Thermodynamic identity (classical):**

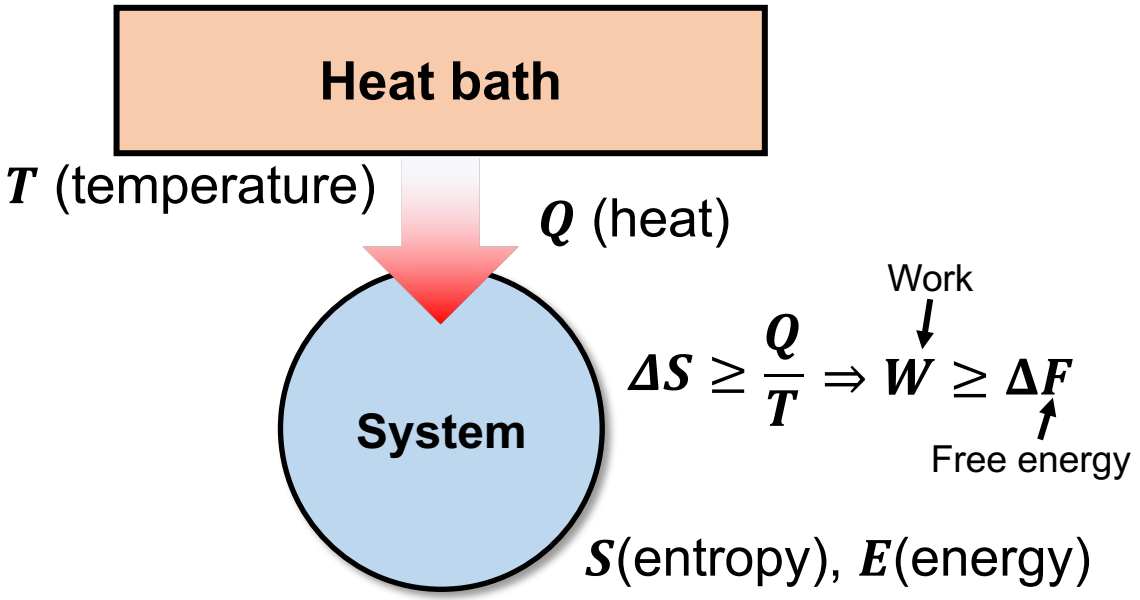
$$\frac{P_{\rightarrow}(\vec{z}_f|\vec{z}_i)}{P_{\leftarrow}(\vec{z}_i^*|\vec{z}_f^*)} = e^{-\beta Q}$$

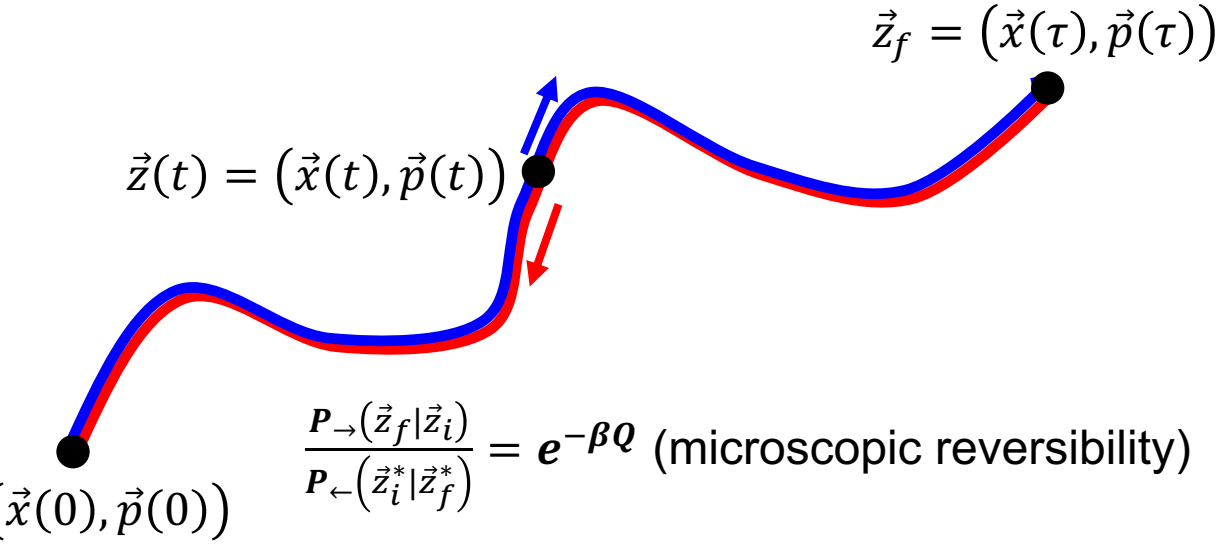
$\vec{z}^* = (\vec{x}, -\vec{p})$: time-reversed coordinate

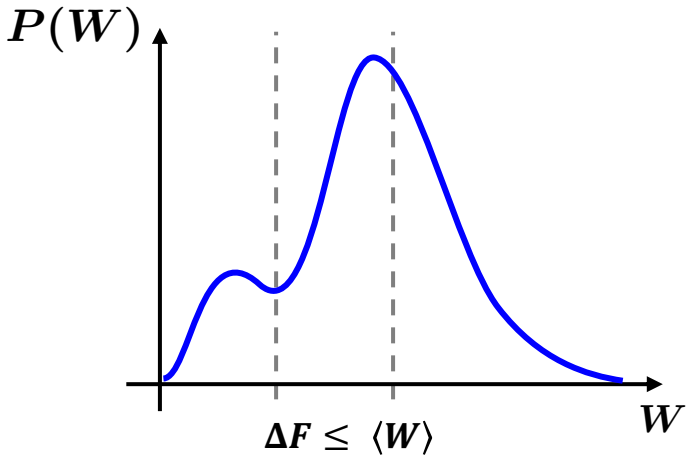
(Microscopic reversibility condition, or detailed balance)

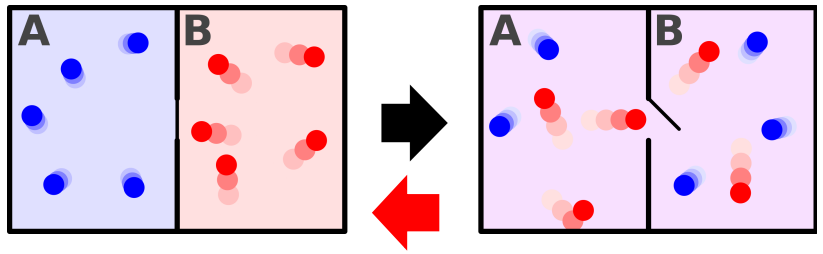
[S. R. de Groot and P. Mazur, *Non-equilibrium Thermodynamics,* (North-Holland, Amsterdam, 1962).]
[R. C. Tolman, Phys. Rev. **23**, 693 (1924); R. C. Tolman, *The Principles of Statistical Mechanics,* (Oxford University Press, London, 1938)]

Microscopic reversibility (classical)









Reverse process is possible but happens with extremely low probability

Fluctuation theorems

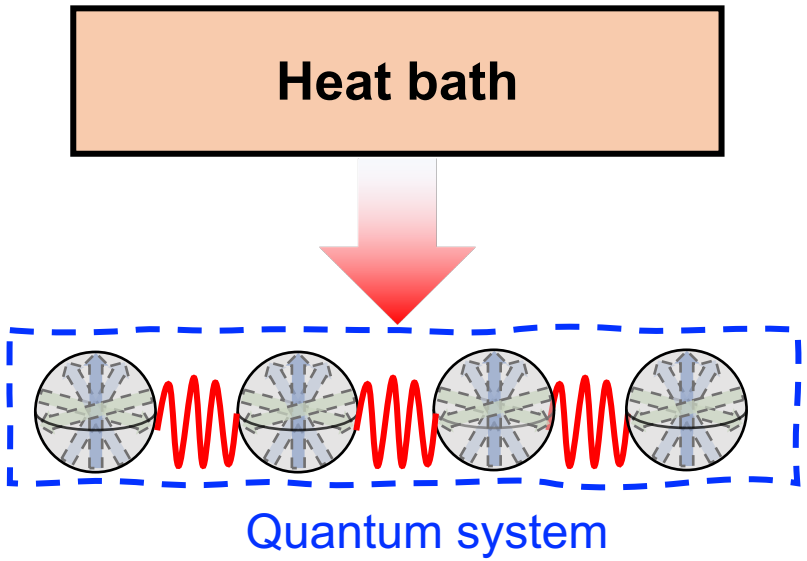
[C. Jarzynski, PRL **78**, 2690 (1997)]

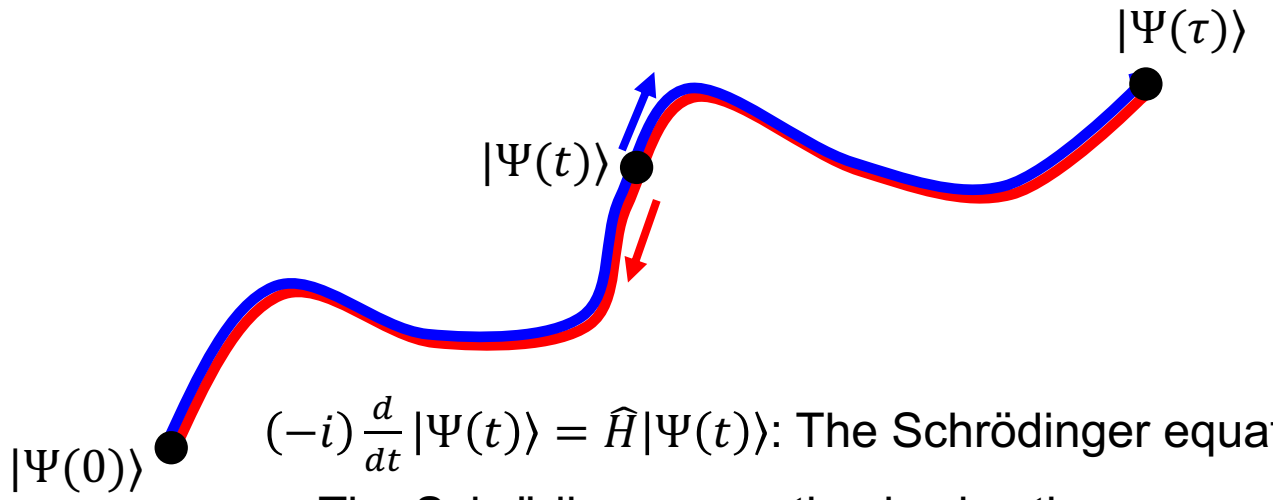
$$\langle e^{-\beta W} \rangle = e^{-\beta \Delta F}$$

[G. E. Crooks, PRE **60**, 2721 (1999)]

Quantum microscopic reversibility condition?

Microscopic reversibility (quantum)





$(-i)\frac{d}{dt}|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle$: The Schrödinger equation

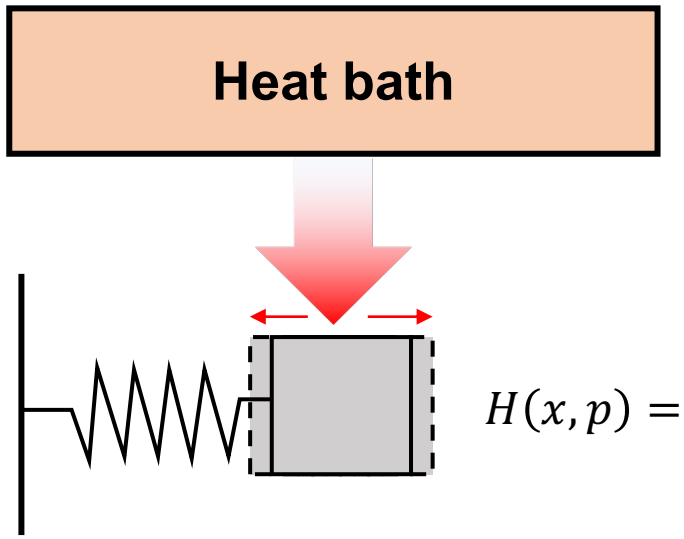
The Schrödinger equation is also time-symmetric

$t \to -t$ & $|\Psi\rangle \to |\Psi^*\rangle$

$$\frac{P_{\rightarrow}}{P_{\leftarrow}} \stackrel{?}{=} e^{-\beta Q}$$

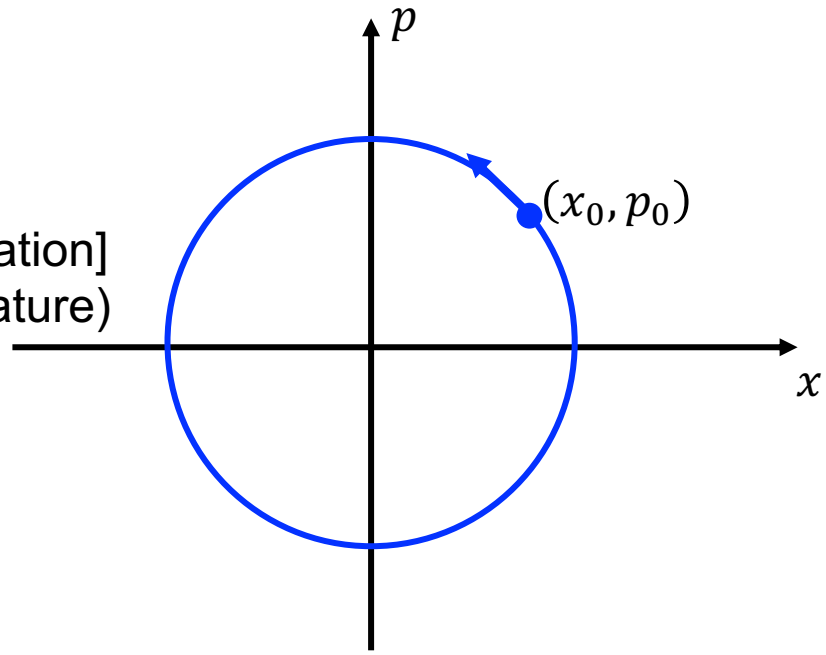
Let's consider a very simple system ➔ a simple harmonic oscillator

Classical harmonic oscillator

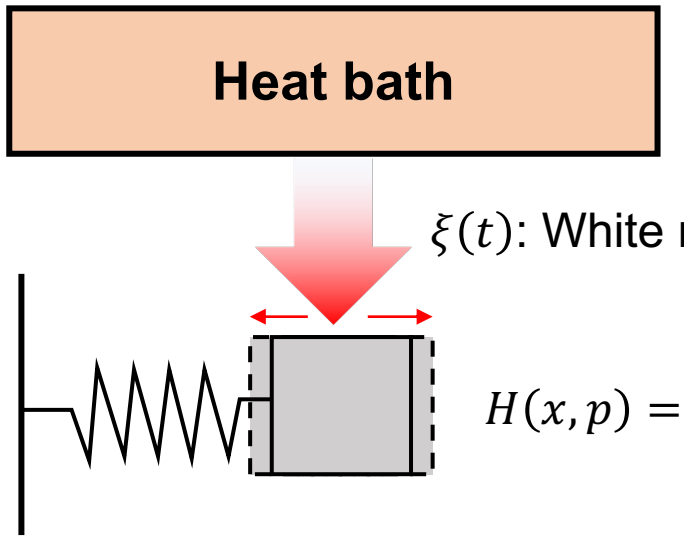


[Without thermalization]
(or at zero temperature)

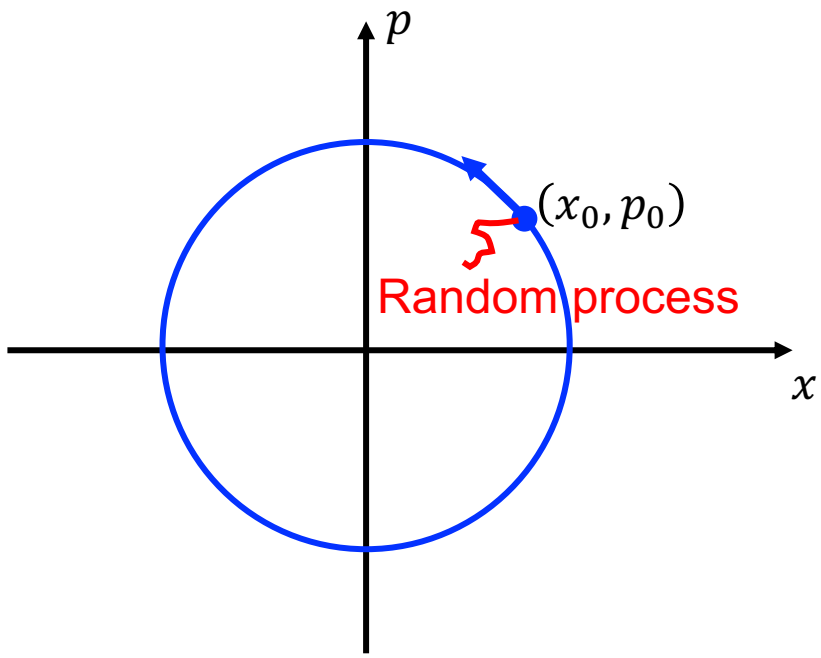
$$H(x,p) = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$$



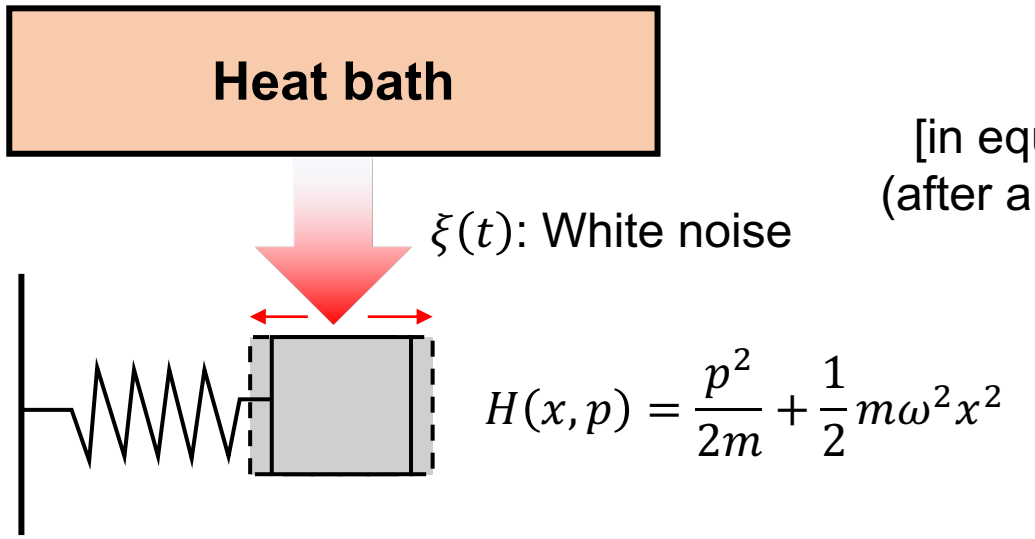
Classical harmonic oscillator



$$H(x,p) = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$$

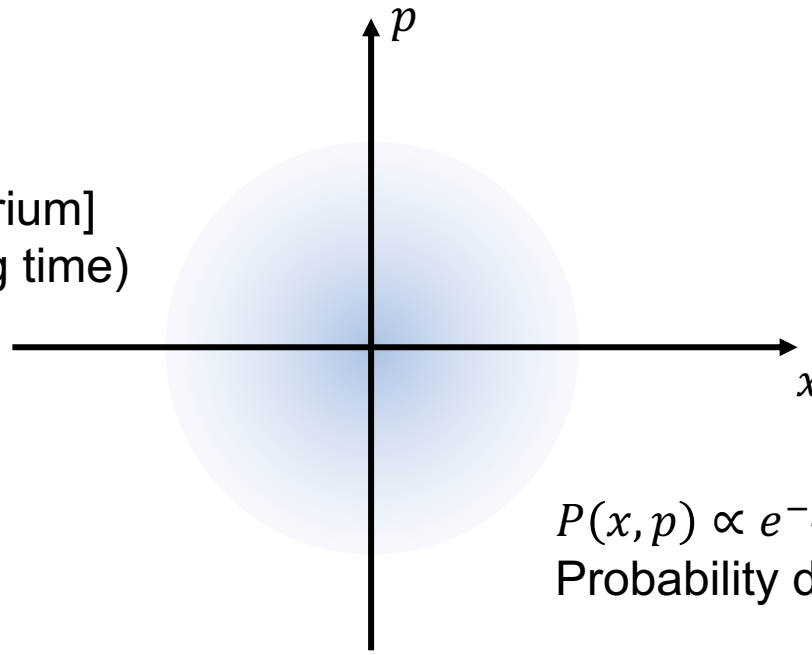


Classical harmonic oscillator



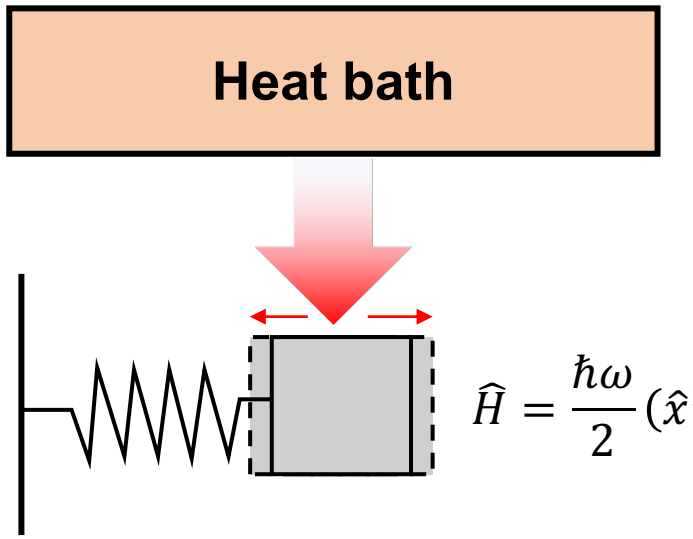
$$H(x,p) = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$$

[in equilibrium]
(after a long time)

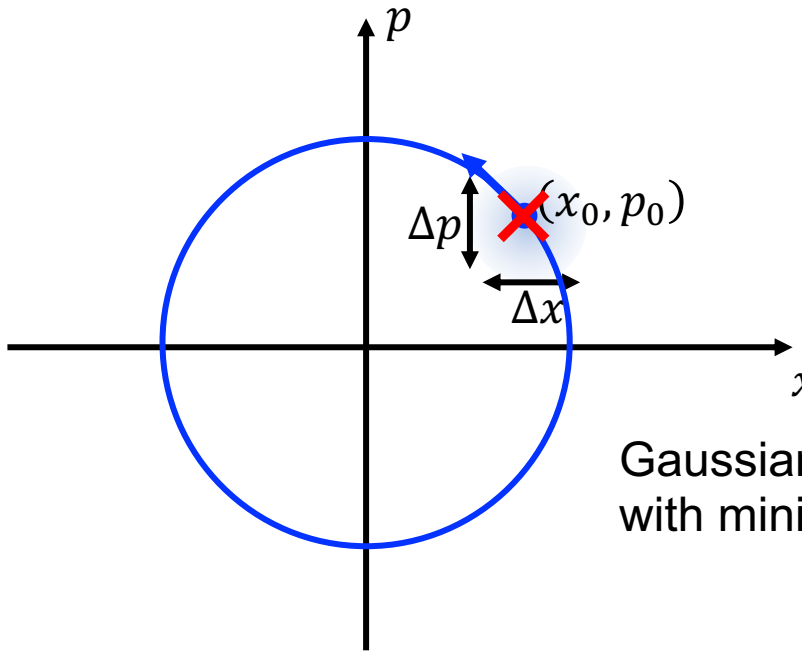


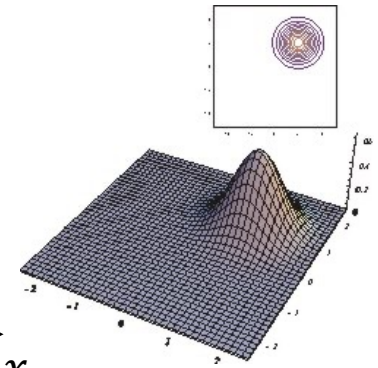
$P(x,p) \propto e^{-\beta H(x,p)}$
Probability density

Quantum harmonic oscillator



$$\hat{H} = \frac{\hbar\omega}{2}(\hat{x}^2 + \hat{p}^2)$$





Gaussian distribution
with minimum uncertainty

However, we cannot precisely determine $\hat{x}$ and $\hat{p}$ simultaneously as they do not commute to each other

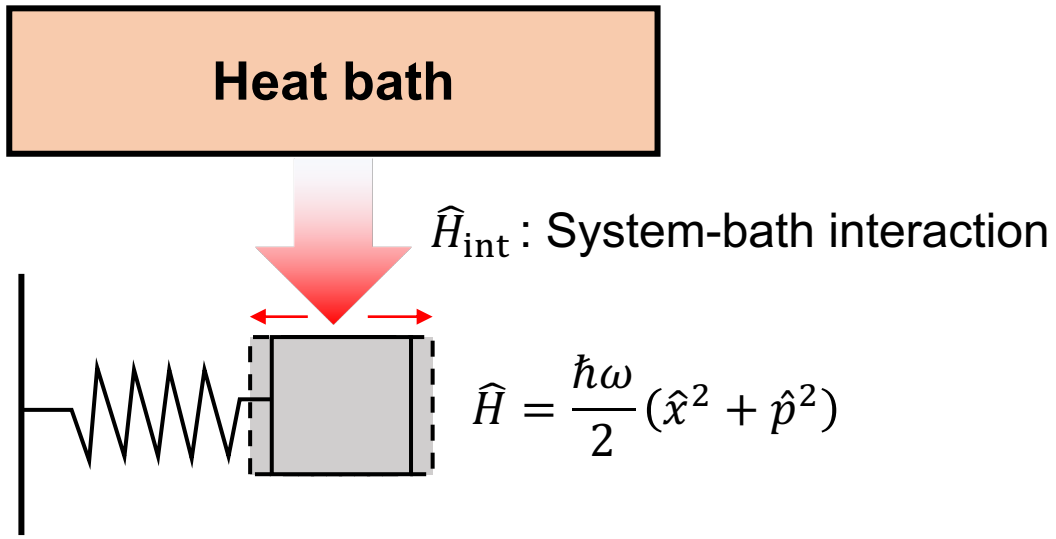
$$[\hat{x}, \hat{p}] = i\hbar \Rightarrow \Delta x \Delta p \geq \hbar/2$$

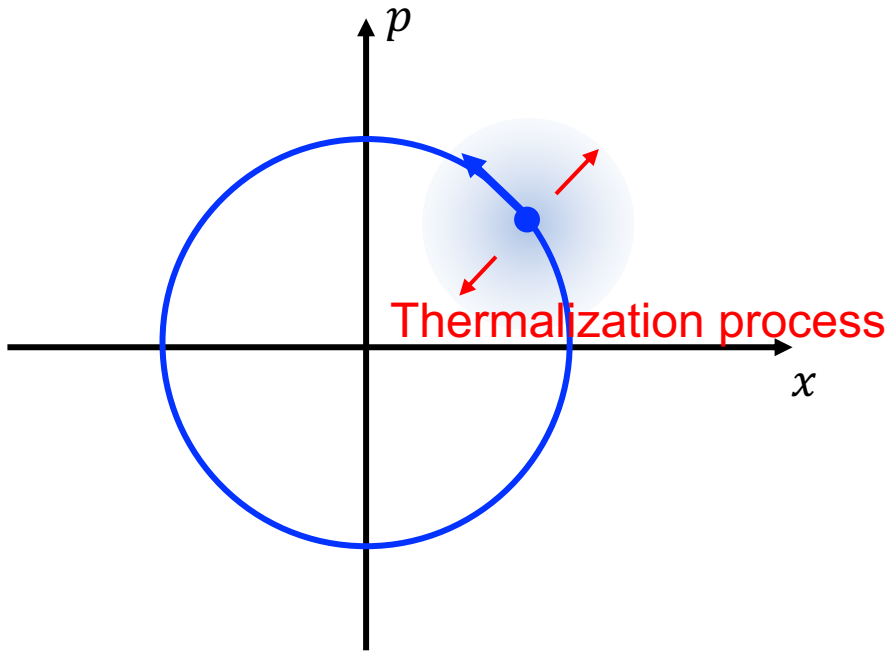
We cannot have a point (x_0, p_0) in phase space as in classical theory

The best choice is using the minimum uncertainty state (a.k.a. coherent states): $|\alpha_0\rangle = |(x_0, p_0)\rangle$

$$|\alpha\rangle = e^{-\frac{|\alpha|^2}{2}} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle$$

Quantum harmonic oscillator





However, we cannot precisely determine $\hat{x}$ and $\hat{p}$ simultaneously as they do not commute to each other

$$[\hat{x}, \hat{p}] = i\hbar \Rightarrow \Delta x \Delta p \geq \hbar/2$$

We cannot have a point (x_0, p_0) in phase space as in classical theory

The best choice is using the minimum uncertainty state (a.k.a. coherent states): $|\alpha_0\rangle = |(x_0, p_0)\rangle$

Will we have the same microscopic reversibility condition as in classical theory?

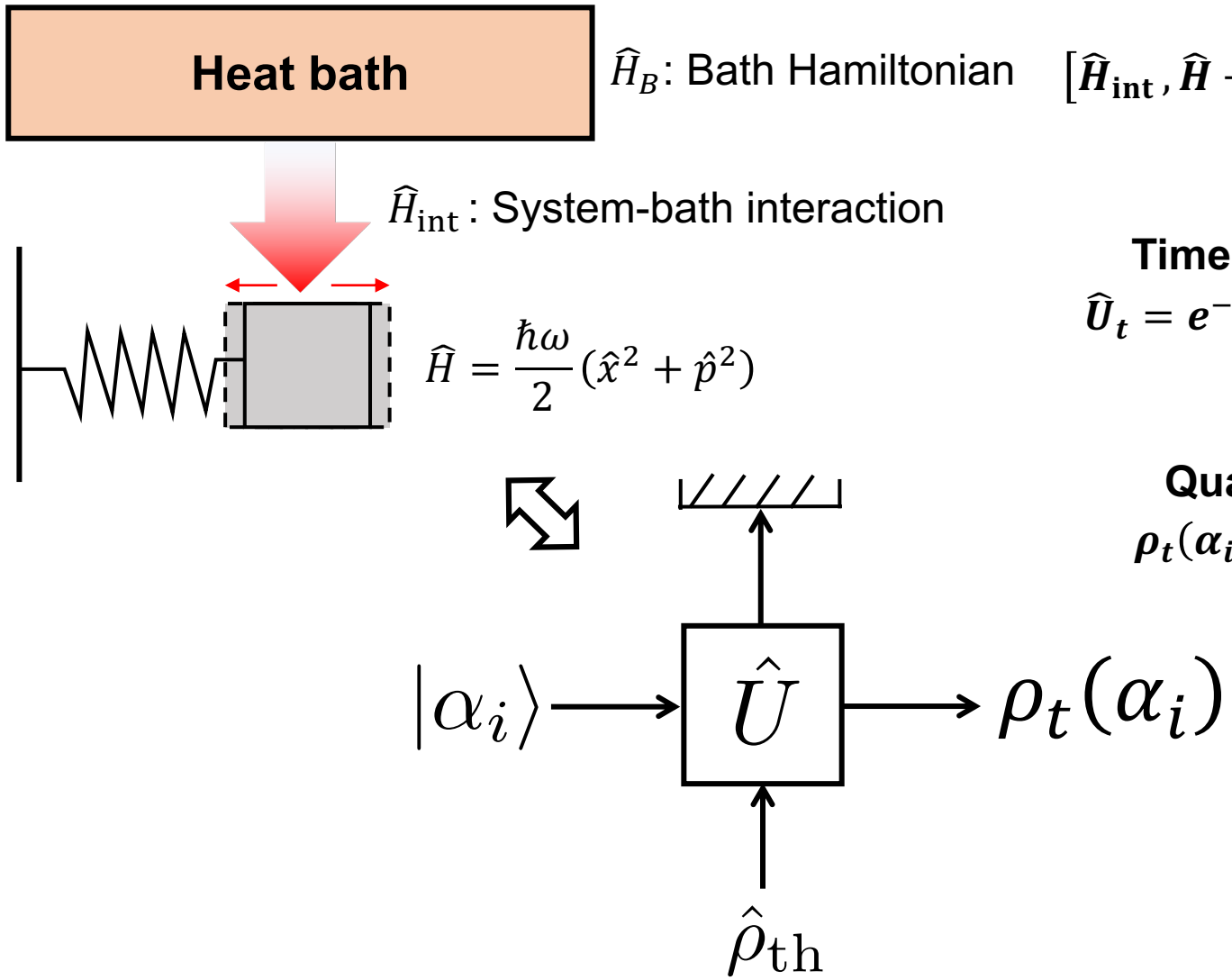
In this talk…

- **Main question:**
  Can we find a fundamental difference between quantum & classical thermodynamic principles?

- **Checklist**

Fundamental thermodynamic principle?	Microscopic reversibility
A simple classical/quantum process?	Thermalization of a harmonic oscillator
What makes the difference?	Uncertainty principle
What is the correction?	
Classical limit?	
How to test it?	

Transition amplitude under thermalization



$[\hat{H}_{\mathrm{int}}, \hat{H} + \hat{H}_B] = 0$: **Energy preservation condition**

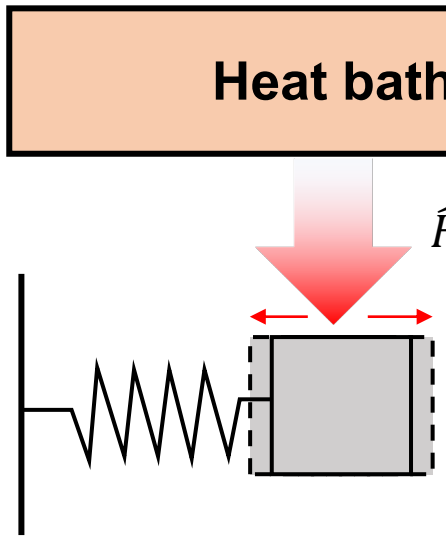
Time-evolution of the total system

$$\hat{U}_t = e^{-i(\hat{H}+\hat{H}_B+\hat{H}_{\mathrm{int}})t} = e^{-i\hat{H}t}e^{-i\hat{H}_B t}e^{-i\hat{H}_{int}t}$$

Quantum state after evolution

$$\rho_t(\alpha_i) = \mathrm{Tr}_{\mathrm{th}}[\hat{U}_t(|\alpha_i\rangle\langle\alpha_i| \otimes \hat{\rho}_{\mathrm{th}})\hat{U}_t^\dagger]$$

Transition amplitude under thermalization



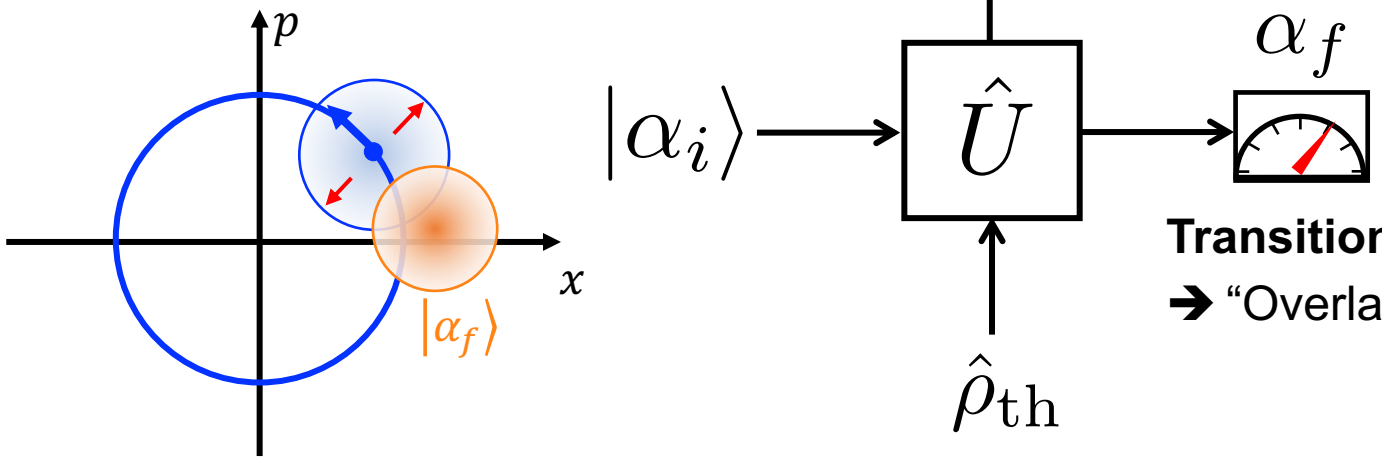
$[\hat{H}_{\mathrm{int}}, \hat{H} + \hat{H}_B] = 0$: **Energy preservation condition**

Time-evolution of the total system

$$\hat{U}_t = e^{-i(\hat{H}+\hat{H}_B+\hat{H}_{\mathrm{int}})t} = e^{-i\hat{H}t}e^{-i\hat{H}_B t}e^{-i\hat{H}_{int}t}$$

Quantum state after evolution

$$\rho_t(\alpha_i) = \mathrm{Tr}_{\mathrm{th}}[\hat{U}_t(|\alpha_i\rangle\langle\alpha_i| \otimes \hat{\rho}_{\mathrm{th}})\hat{U}_t^\dagger]$$



Transition amplitude: $P(\alpha_f|\alpha_i)$

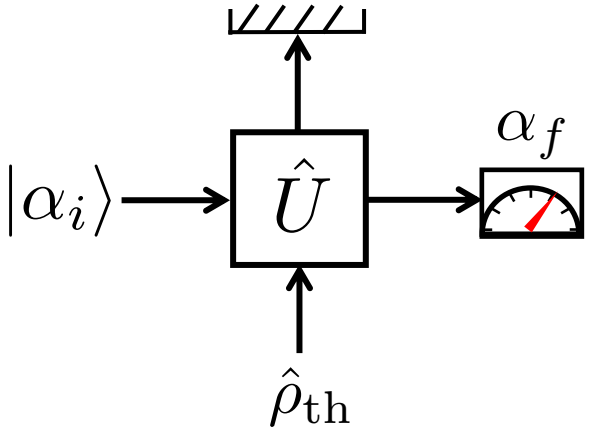
➔ "Overlap" between the final state and coherent state $|\alpha_f\rangle$

$$P(\alpha_f|\alpha_i) \propto \langle\alpha_f|\rho_t(\alpha_i)|\alpha_f\rangle$$

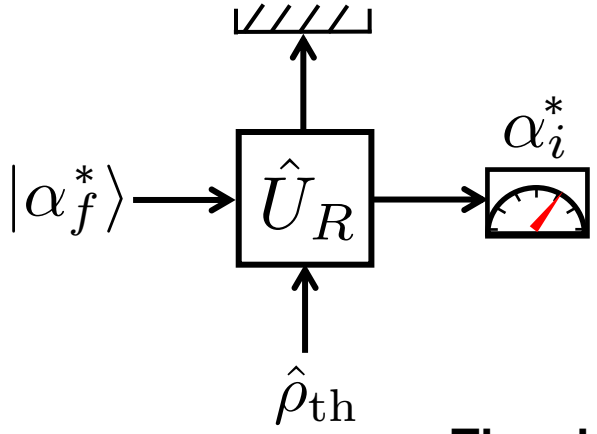
Also known as "Husimi Q function"

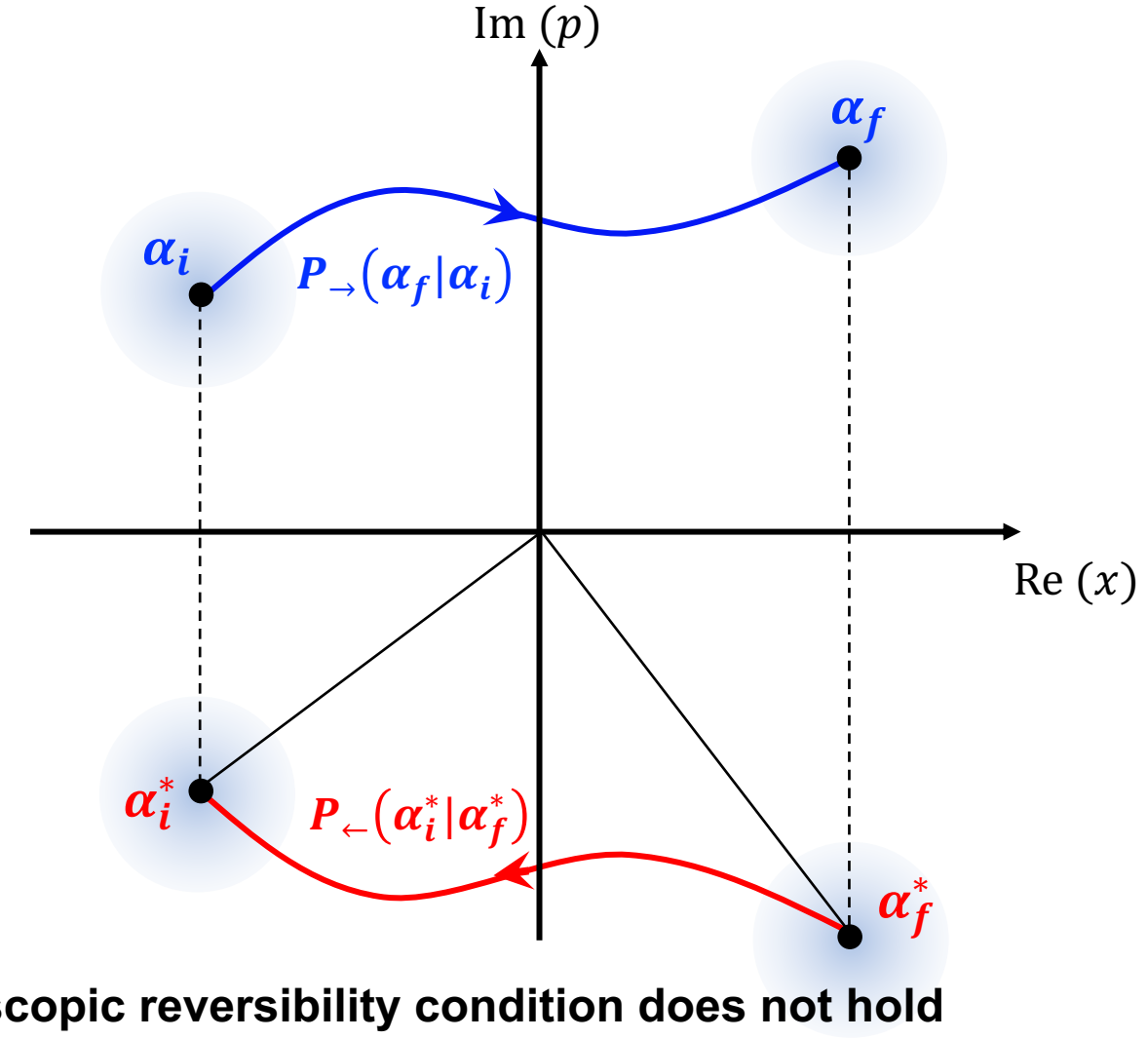
Quantum modification of microscopic reversibility

[Forward process]



[Backward process]





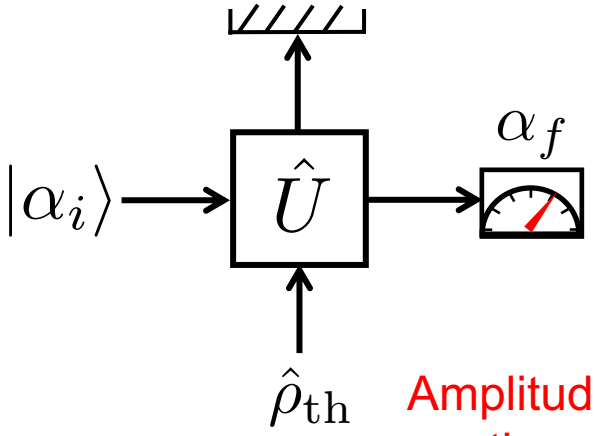
The classical microscopic reversibility condition does not hold

$$\frac{\boldsymbol{P_{\rightarrow}(\alpha_f|\alpha_i)}}{\boldsymbol{P_{\leftarrow}(\alpha_i^*|\alpha_f^*)}} \neq \boldsymbol{e^{-\beta Q}}$$

➔ **We need some quantum modification!**

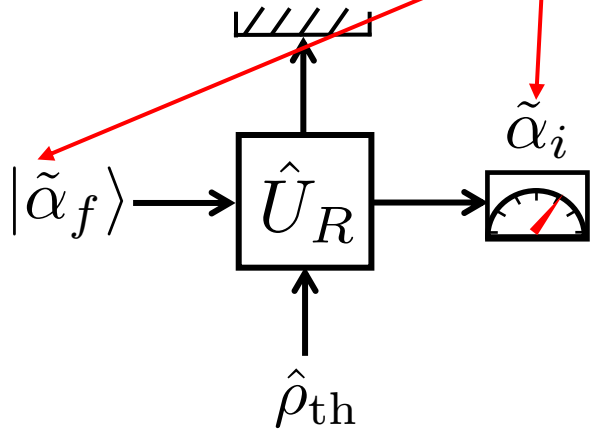
Quantum modification of microscopic reversibility

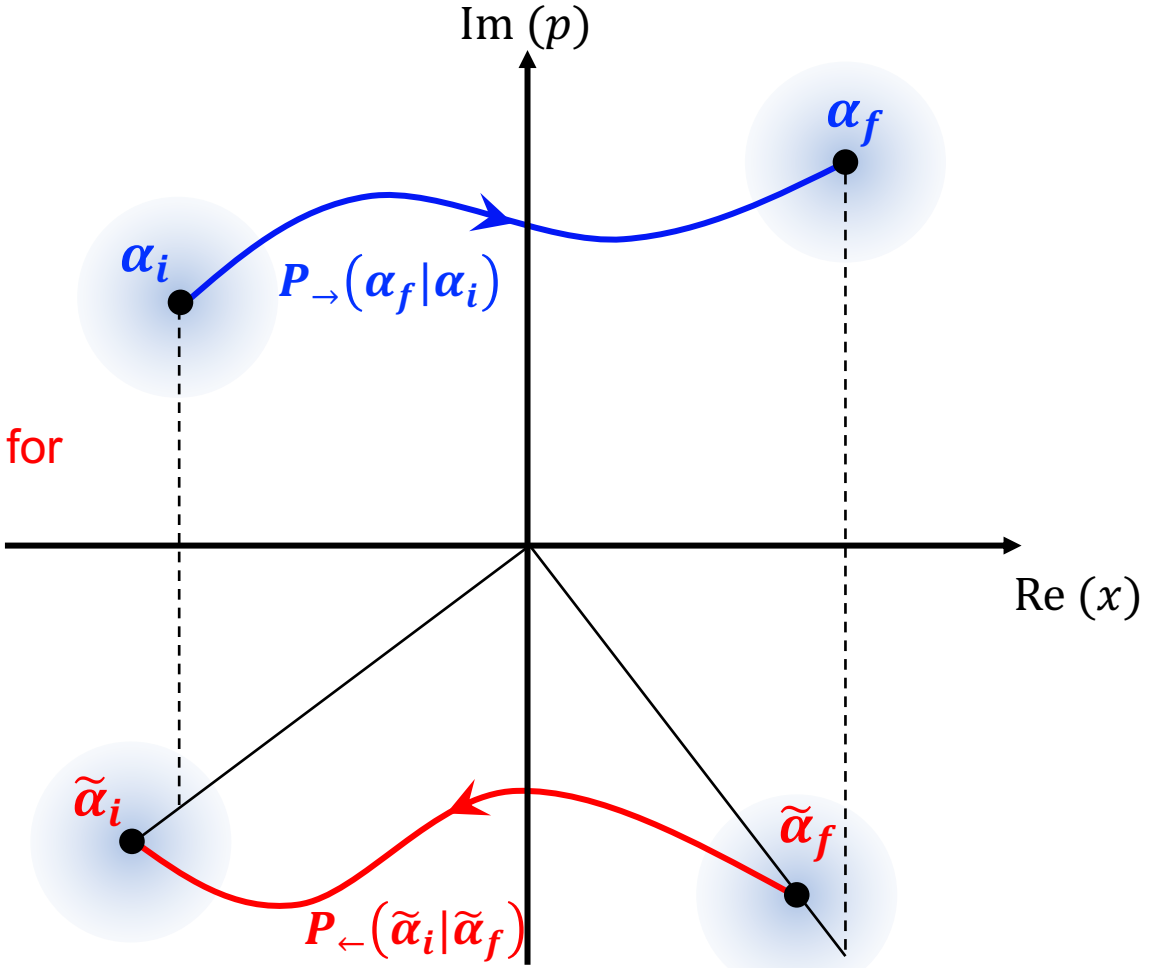
[Forward process]



Amplitudes are **rescaled** for the reverse process!

[Backward process]





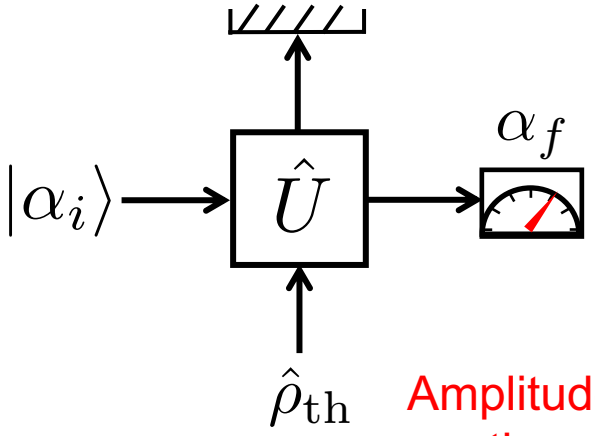
$|\alpha\rangle = e^{-\frac{|\alpha|^2}{2}} \sum_{n=0}^{\infty} \frac{\alpha^n}{\sqrt{n!}} |n\rangle$, $\hat{H} = \frac{\hbar\omega_0}{2}(\hat{x}^2 + \hat{p}^2)$

: Contains coherence between different energy states $|n\rangle$

➔ Different energies should be weighted differently!

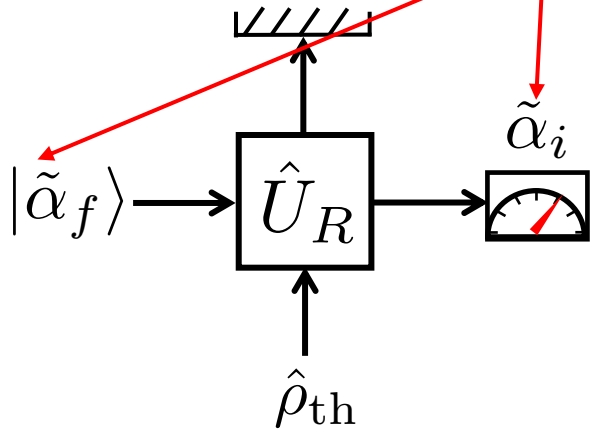
Quantum modification of microscopic reversibility

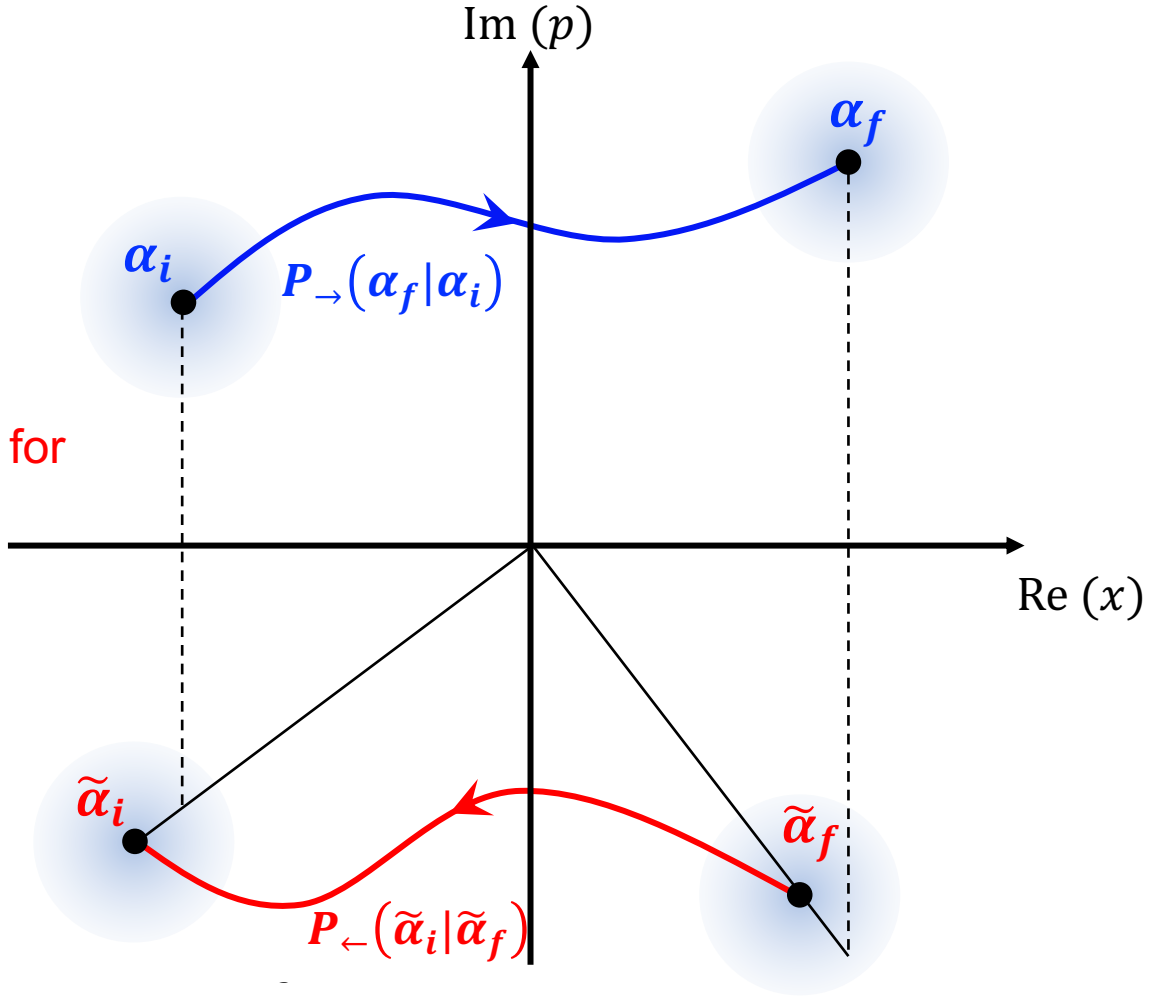
[Forward process]



Amplitudes are **rescaled** for the reverse process!

[Backward process]





$$\frac{P_{\rightarrow}(\alpha_f|\alpha_i)}{P_{\leftarrow}(\tilde{\alpha}_i|\tilde{\alpha}_f)} = \exp\left[-\frac{|\alpha_f|^2}{n_{\mathrm{th}}+1}+\frac{|\alpha_i|^2}{n_{\mathrm{th}}}\right] = \Upsilon e^{-\beta Q}$$: Quantum microscopic reversibility

Quantum correction

In this talk…

- **Main question:**
  Can we find a fundamental difference between quantum & classical thermodynamic principles?

- **Checklist**

Fundamental thermodynamic principle?	Microscopic reversibility
A simple classical/quantum process?	Thermalization of a harmonic oscillator
What makes the difference?	Uncertainty principle
What is the correction?	Rescaling / Correction term
Classical limit?	
How to test it?	

In this talk…

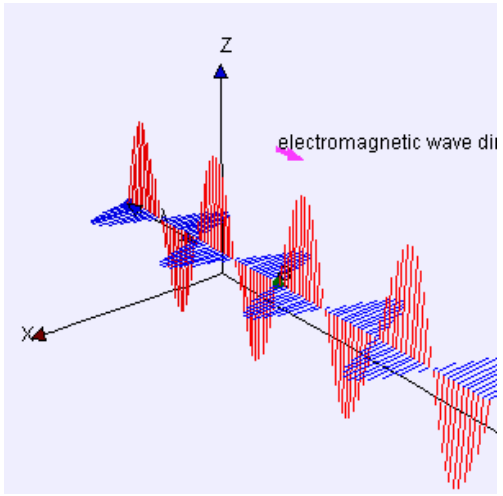
- **Main question:**
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Classical limit?	
How to test it?	Using quantum optics

Experimental demonstration using quantum optics

- **Electromagnetic wave as a harmonic oscillator**



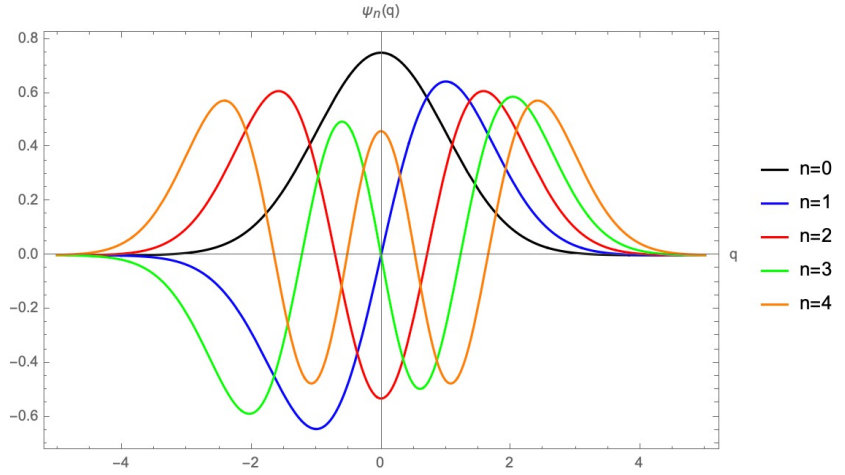
$$H = \frac{1}{2}(q^2 + p^2)$$

"Harmonic oscillator"

(we take $\omega = 1$ for simplicity)

$$[\hat{q}, \hat{p}] = \hat{q}\hat{p} - \hat{p}\hat{q} = i$$

$$\hat{H} = \frac{1}{2}(\hat{q}^2 + \hat{p}^2)$$

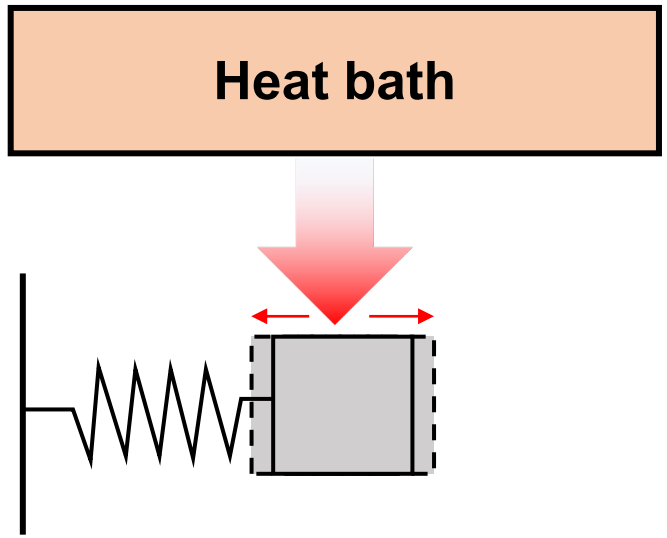


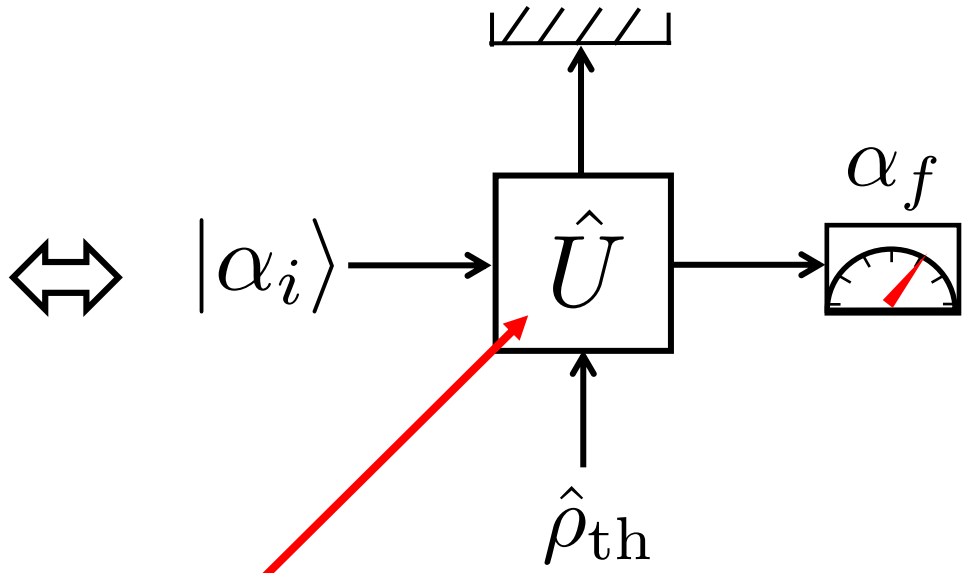
➔ $E_n = n + \frac{1}{2}$ (Quantization)

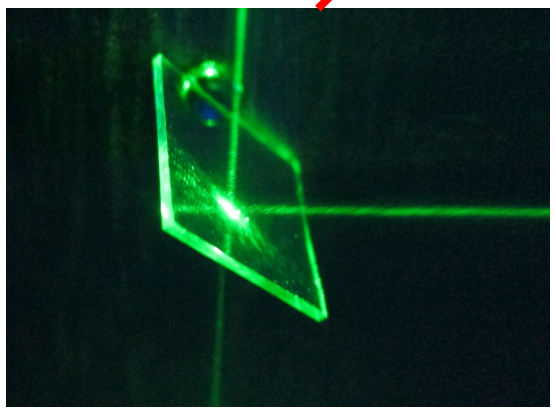
[n : Photon number]

Coherent states are easy to prepare & measure!
(noting but laser)

Experimental demonstration using quantum optics



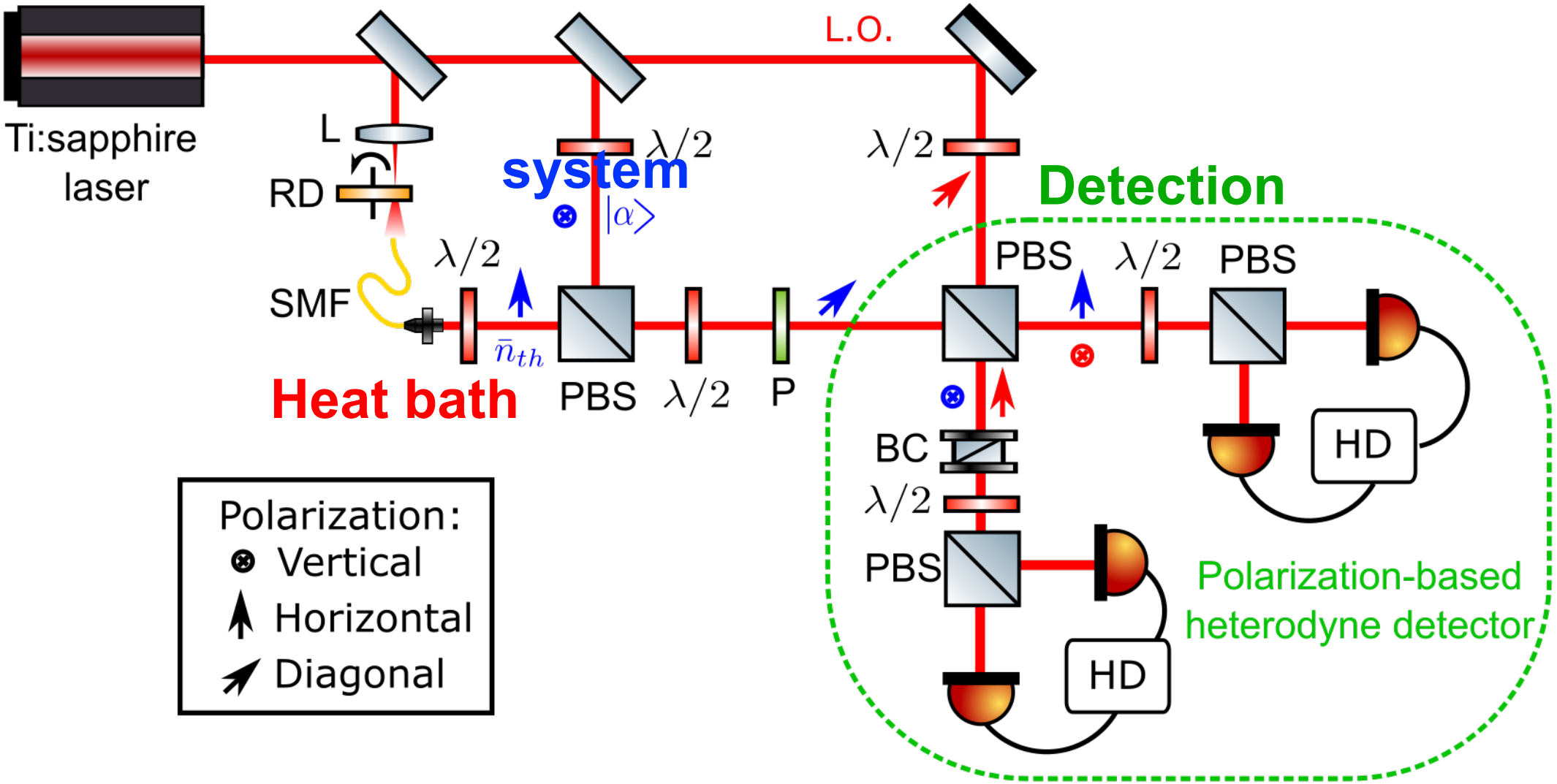




System-bath interaction can be realized by beam-splitter (half-transparent mirror)

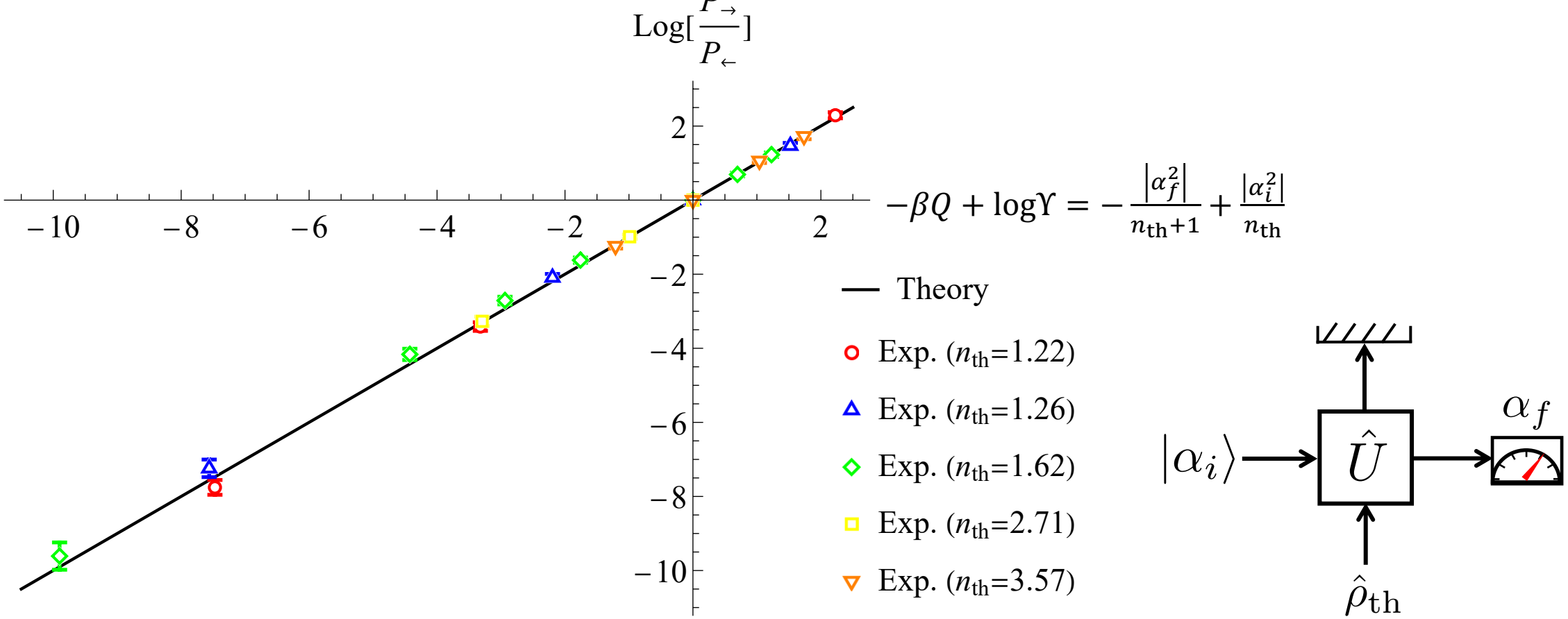
Experimental demonstration using quantum optics

Experimental collaboration with Marco Bellini's group at CNR-INO (Univ. Firenze)



Experimental demonstration using quantum optics

$$\frac{P_{\rightarrow}(\alpha_f|\alpha_i)}{P_{\leftarrow}(\tilde{\alpha}_i|\tilde{\alpha}_f)} = \exp\left[-\frac{|\alpha_f|^2}{n_{\mathrm{th}}+1}+\frac{|\alpha_i|^2}{n_{\mathrm{th}}}\right] = \Upsilon e^{-\beta Q}$$: **Quantum microscopic reversibility**



Holds for any choices of α_i, α_f, n_{th} and the beam splitter reflectivity (interaction strength)!

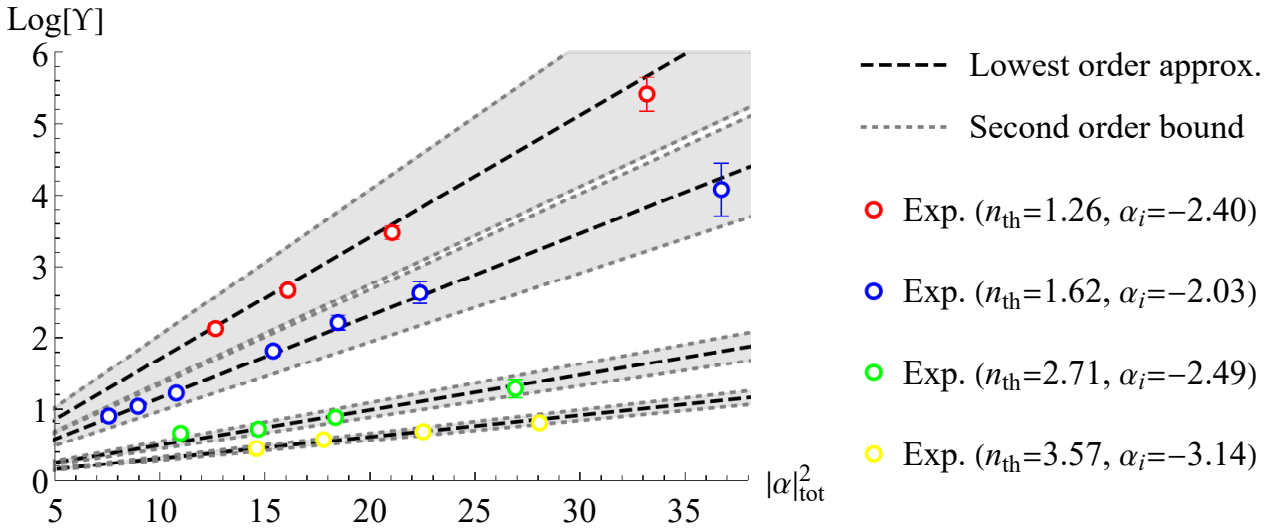
Experimental demonstration using quantum optics

$$\frac{P_{\rightarrow}(\alpha_f|\alpha_i)}{P_{\leftarrow}(\tilde{\alpha}_i|\tilde{\alpha}_f)} = \exp\left[-\frac{|\alpha_f|^2}{n_{\mathrm{th}}+1}+\frac{|\alpha_i|^2}{n_{\mathrm{th}}}\right] = \Upsilon e^{-\beta Q}$$ **: Quantum microscopic reversibility**

Υ: Quantum correction

Deviation from the classical theory: $\log[\Upsilon] \approx \frac{(\beta\hbar\omega_0)^2}{2}|\alpha|^2_{\mathrm{tot}}$

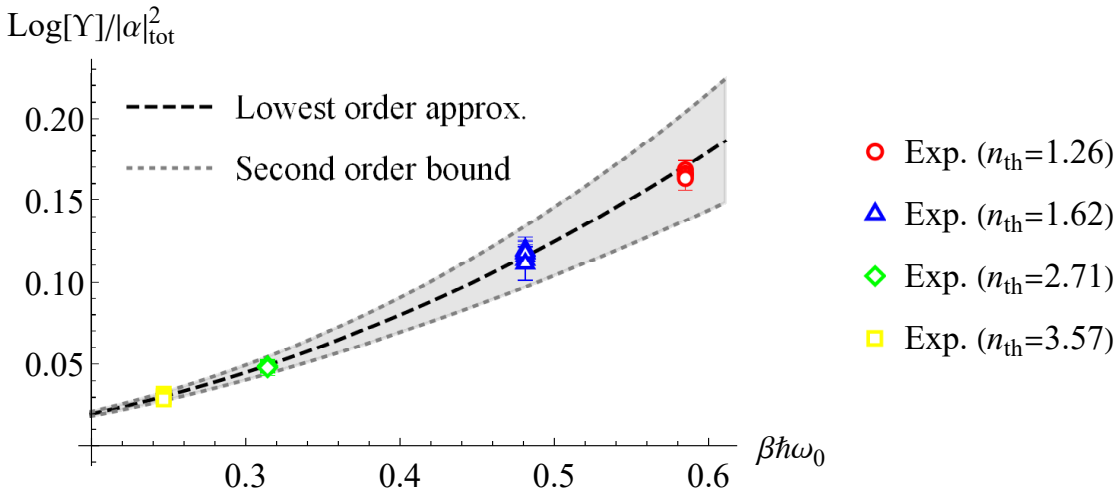
- Linearly increase with the total coherence $|\alpha|^2_{\mathrm{tot}} = |\alpha_i|^2 + |\alpha_f|^2$
- Quadratically increase with the inverse temperature $\beta\hbar\omega_0$



Quantum correction increases when $|\alpha_i|$&$|\alpha_f|$ increases

$$|\alpha\rangle = e^{-\frac{|\alpha|^2}{2}}\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}|n\rangle$$

The larger the $|\alpha|$, the larger the coherence
(More generally, quantum fisher information)



Quantum to classical transition
when the temperature becomes high
$(\beta = \frac{1}{k_B T} \approx 0$ or $n_{\mathrm{th}}, T \gg 1)$

For more detail: PRL **129**, 17064 (2022).
APS Physics Synopsis “Microscopic Reversibility Goes Quantum”

In this talk…

- **Main question:**
  Can we find a fundamental difference between quantum & classical thermodynamic principles?

- **Checklist**

Fundamental thermodynamic principle?	Microscopic reversibility
A simple classical/quantum process?	Thermalization of a harmonic oscillator
What makes the difference?	Uncertainty principle
What is the correction?	Rescaling / Correction term
Classical limit?	High temperature, small coherence
How to test it?	Using quantum optics

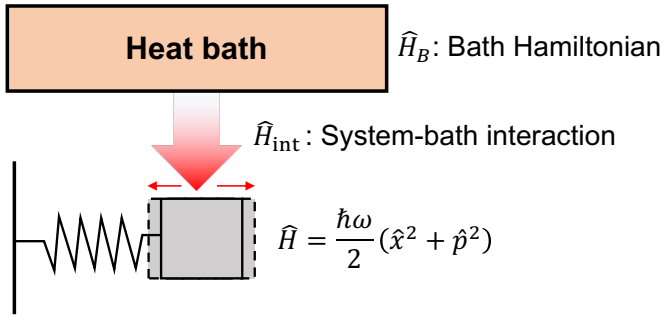
Remarks

- Thermodynamic principles in quantum mechanics can be fundamentally different
  - ➢ In quantum mechanics, phase space cannot be sharply determined (∵ **uncertainty relation**)
    ➔ Best choice: coherent states (for a quantum harmonic oscillator system)
  - ➢ Quantum modification of the microscopic reversibility condition can be found & experimentally tested

$$\frac{P_{\rightarrow}(\alpha_f|\alpha_i)}{P_{\leftarrow}(\tilde{\alpha}_i|\tilde{\alpha}_f)} = \exp\left[-\frac{|\alpha_f|^2}{n_{\mathrm{th}}+1}+\frac{|\alpha_i|^2}{n_{\mathrm{th}}}\right] = \Upsilon e^{-\beta Q}$$

"Rescaling"

Quantum correction

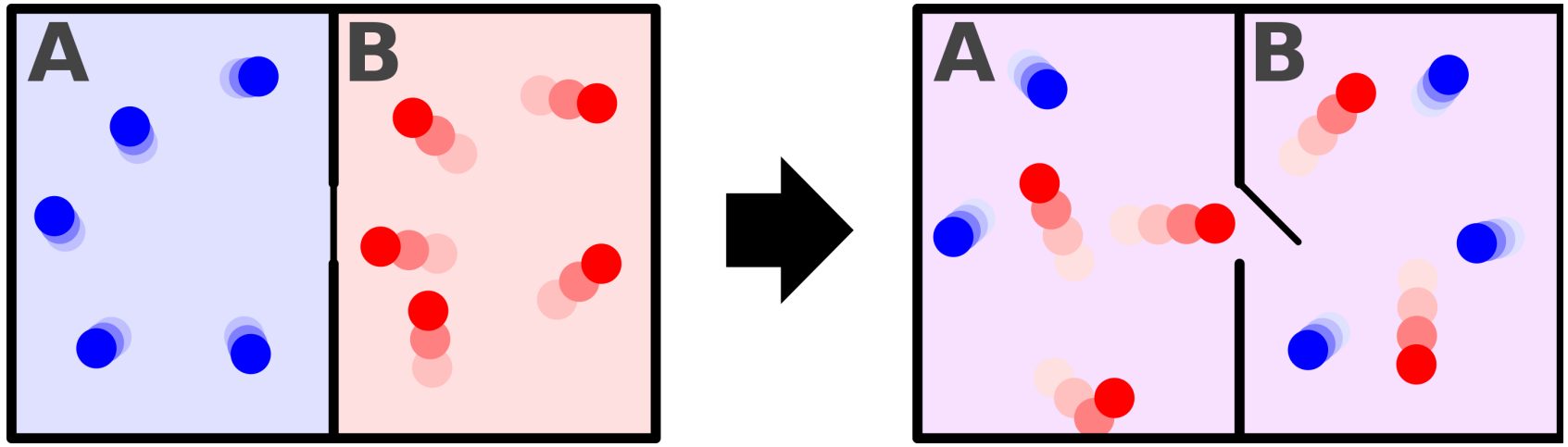


Quantum effects contribute severely for the system with large coherence & bath at low temperature

- Possible applications
  - ➢ Strong symmetry between forward/backward processes in thermal contact
    ➔ Noise characterization, evaluating quantum channel capacity
  - ➢ Generalization to any quantum process [HK and M. S. Kim, PRX (2019)]
    ➔ Time-reversal in open quantum dynamics [HK, R. Mukherjee, and M. S. Kim, PRL (2022)]

Thank you

Laws of thermodynamics



- **1st law:** $\Delta E = Q + W$ (system's internal energy; heat; work (done "to" the system)) ➔ Conservation of (total) energy in the closed-system

- **2st law:** Many (but equivalent) versions (Carnot, Clausius, Kelvin, Planck …)

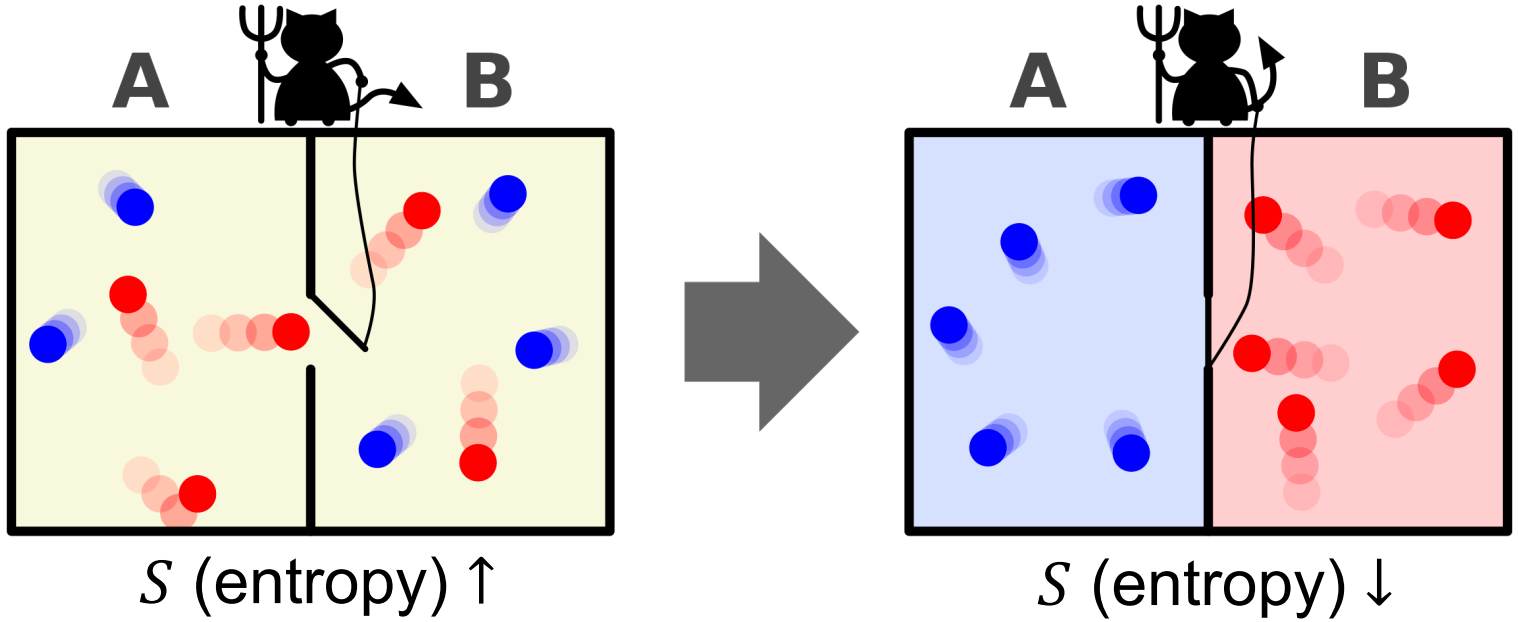
  "Heat can never pass from a colder to a warmer body without some other change"
  "Perpetual motion machine is impossible"
  *"**Entropy** of the entire universe should always increase"*

Maxwell's demon

- **2st law:** Many (but equivalent) versions (Carnot, Clausius, Kelvin, Planck …)

  "Heat can never pass from a colder to a warmer body without some other change"
  "Perpetual motion machine is impossible"
  *"**Entropy** of the entire universe should always increase"*

- **Violation of the second law?**

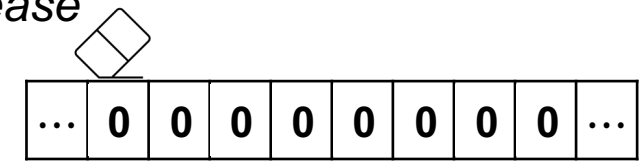


Entropy decreased! (seemingly without any work)

Maxwell's demon

- **2st law:** Many (but equivalent) versions (Carnot, Clausius, Kelvin, Planck …)
  - *"Heat can never pass from a colder to a warmer body without some other change"*
  - *"Perpetual motion machine is impossible"*
  - *"**Entropy** of the entire universe should always increase"*

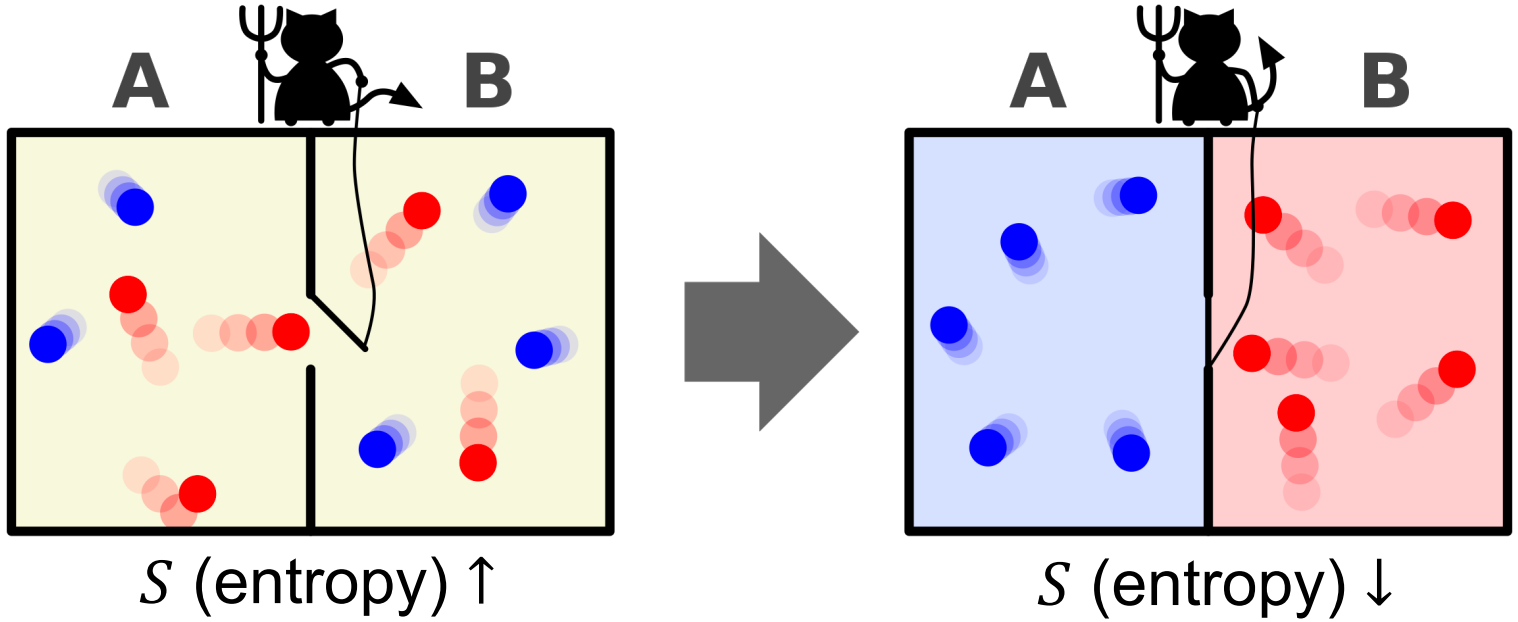
- **Violation of the second law?**



Landauer's principle

$E_{erase} \geq k_B T \log 2$

(per bit)

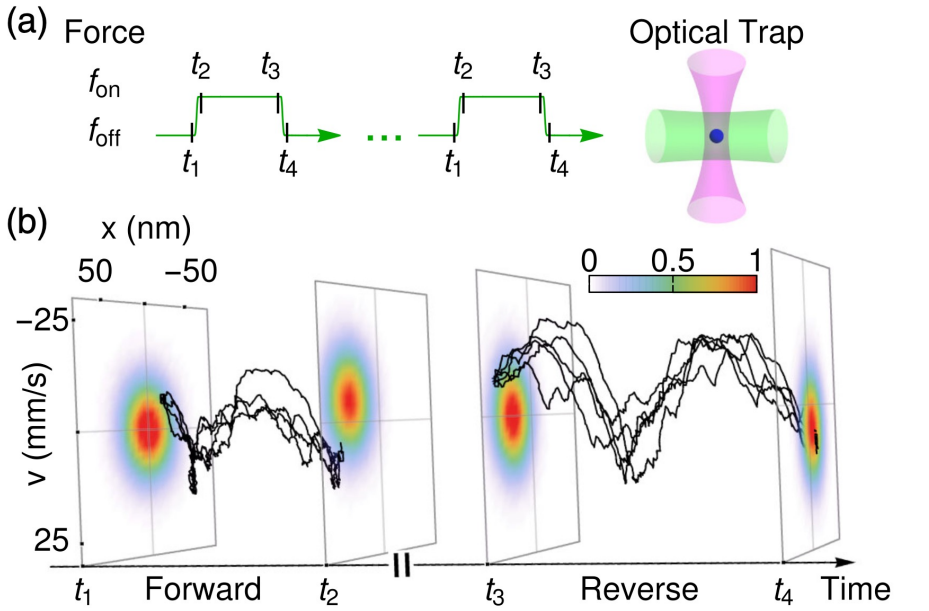


S (entropy) ↑ S (entropy) ↓

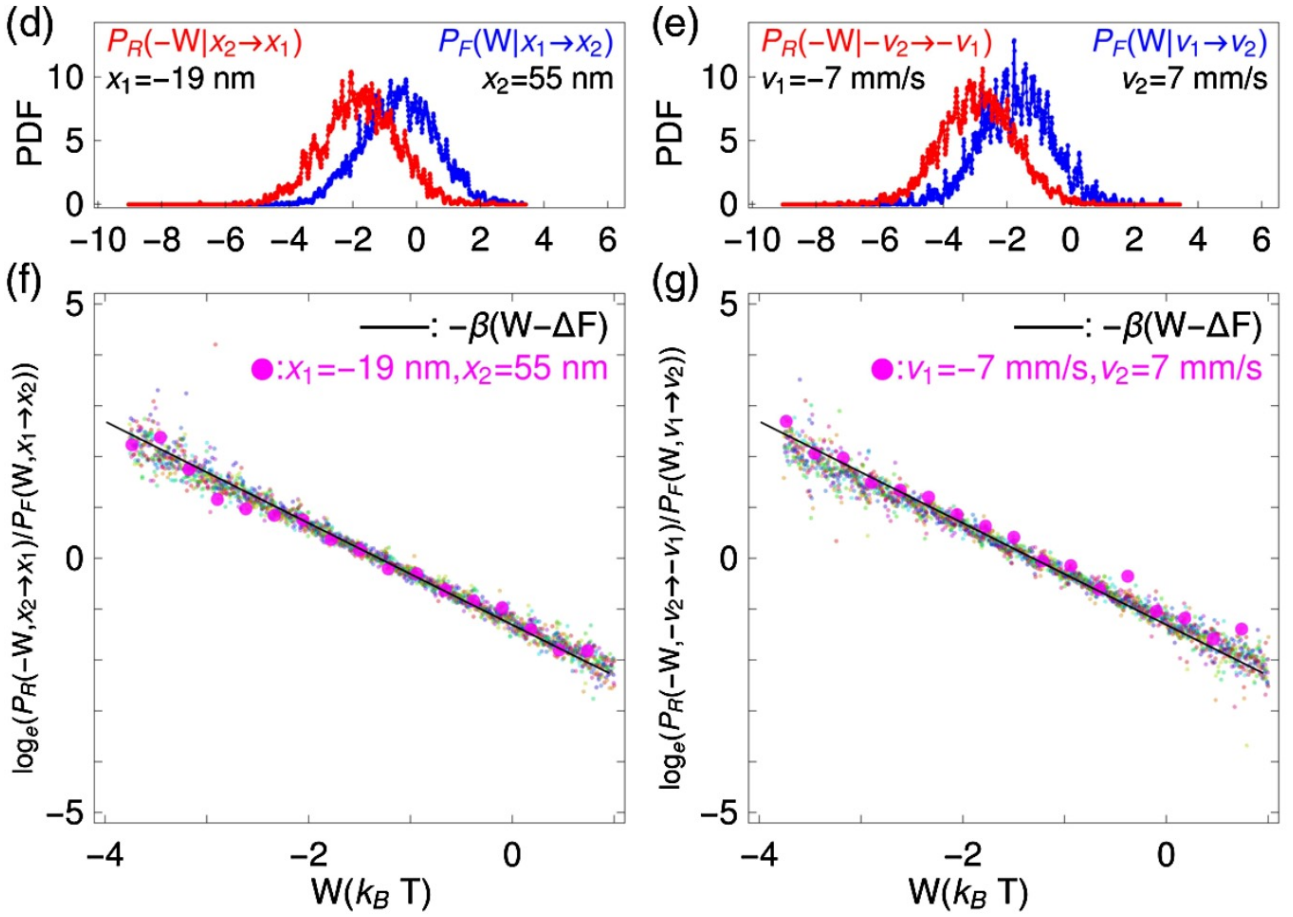
Entropy decreased! (But additional work is needed to erase the memory)

Testing fluctuation theorem in classical thermodynamics

- Recent optical trap experiment



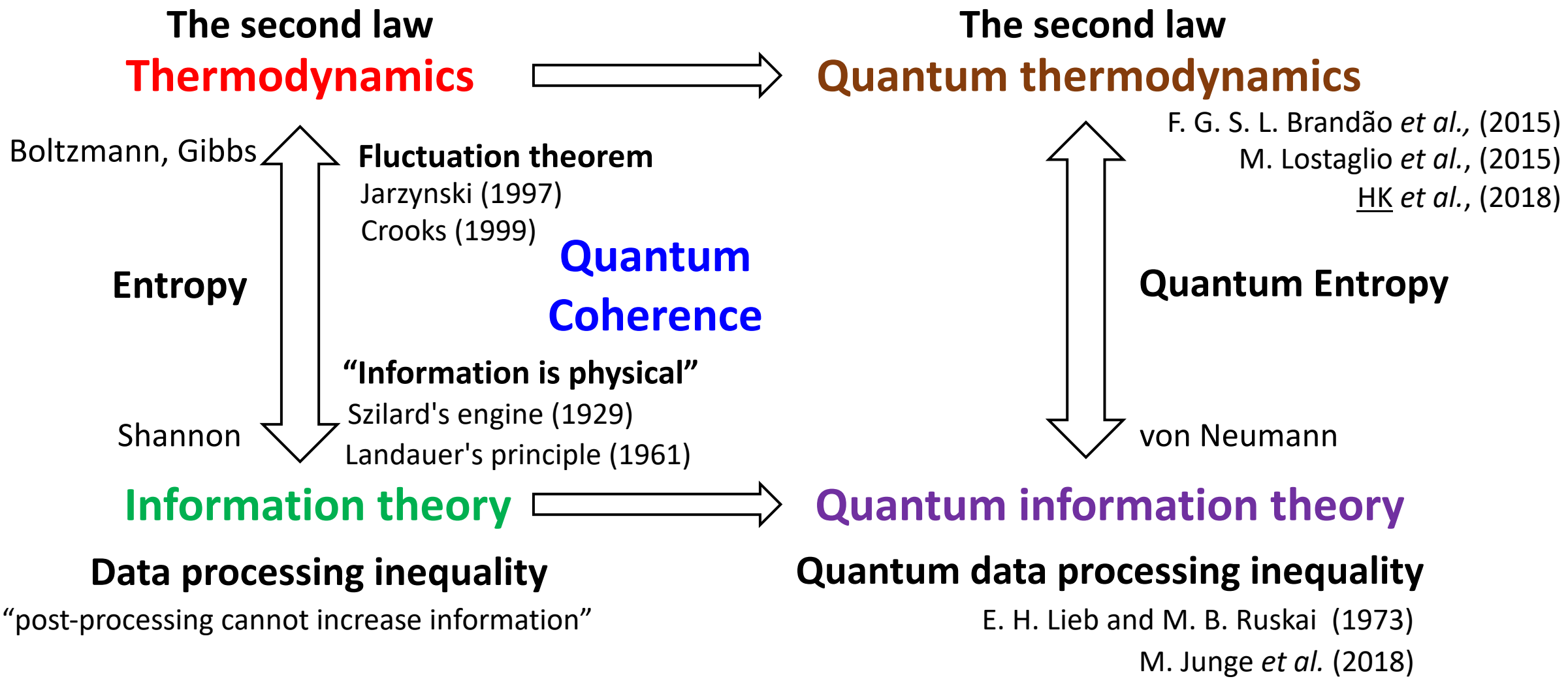
[Phys. Rev. Lett. **120**, 080602 (2018)]



- Main challenges
  - ✓ Precise control of microscopic system
  - ✓ Sufficiently many trajectories should be collected to get “probability distributions”

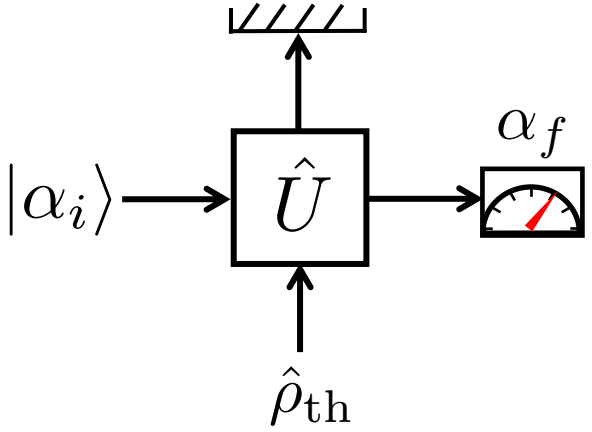
$$\frac{P_{\rightarrow}(\Sigma)}{P_{\leftarrow}(-\Sigma)} = e^{\Sigma} \Leftrightarrow \log\left[\frac{P_{\leftarrow}(-\Sigma)}{P_{\rightarrow}(\Sigma)}\right] = -\beta\Sigma = -\beta(W-\Delta F)$$

Quantum information theory and thermodynamics



Quantum modification of microscopic reversibility

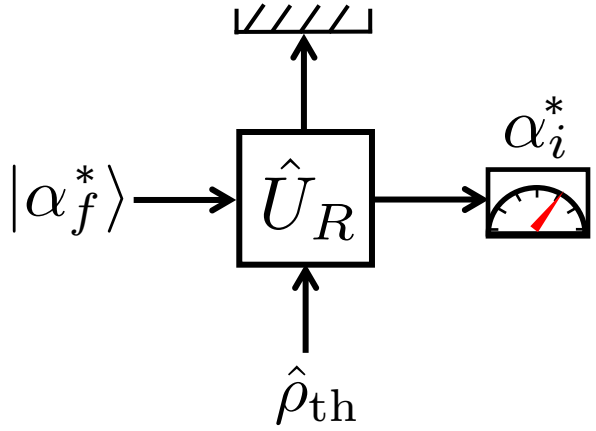
[Forward process]



1. A quantum system is initially prepared in $|\alpha_i\rangle$.
2. The system evolves under a unitary interaction $\hat{U}$ with a thermal bath $\hat{\rho}_{\mathrm{th}}$.
3. We then measure the overlap between the final state and $|\alpha_f\rangle$

Transition probability then leads to $P_{\rightarrow}(\alpha_f|\alpha_i) = \mathrm{Tr}\left[\hat{U}(|\alpha_i\rangle\langle\alpha_i| \otimes \hat{\rho}_{\mathrm{th}})\hat{U}^{\dagger}(|\alpha_f\rangle\langle\alpha_f| \otimes \mathbb{I})\right]$

[Backward process]



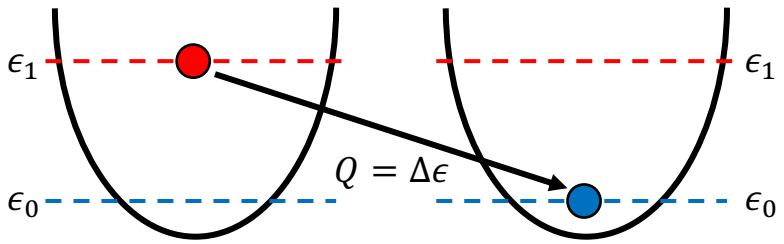
❖ Repeat 1-3 with the time-reversed initial/final states and unitary interaction $\hat{U}_R$.

Transition probability then leads to $P_{\leftarrow}(\alpha_i^*|\alpha_f^*) = \mathrm{Tr}\left[\hat{U}_R(|\alpha_f^*\rangle\langle\alpha_f^*| \otimes \hat{\rho}_{\mathrm{th}})\hat{U}_R^{\dagger}(|\alpha_i^*\rangle\langle\alpha_i^*| \otimes \mathbb{I})\right]$

Quantum entropy production

- Consider a two-level system

[Classical]



$$S = \langle -\log(p) \rangle_p = \sum_i p_i \, (-\log p_i)$$

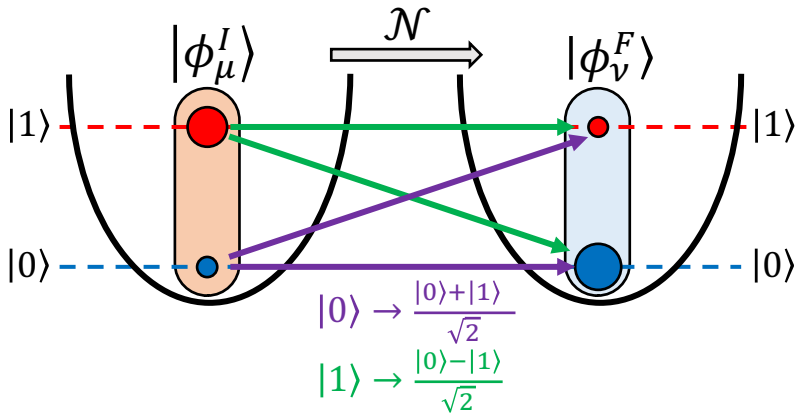
$$E = \langle H \rangle_p = \sum_i p_i \, H_i$$

$$W = 0 \;\rightarrow\; Q = \Delta E$$

Both entropy and heat are obtained from the same distribution p_i

$$\boldsymbol{\Sigma = \Delta S - \beta \Delta E}$$

[Quantum]



$$S = \langle -\log \rho \rangle_\rho \;\rightarrow\; \hat{S} = -\sum_\mu \log p_\mu \, |\phi_\mu\rangle\langle\phi_\mu|$$

$$E = \langle \hat{H} \rangle_\rho \;\rightarrow\; \hat{H} = \sum_i E_i \, |i\rangle\langle i|$$

Eigenstate of ρ

Energy eigenstate

$$\boldsymbol{\Sigma = \Delta S - \beta \Delta E}$$

but $\hat{S}$ and $\hat{H}$ may not commute in QM!

Quantum entropy production

- Quasi-probability distribution of quantum entropy production

$S = \langle -\log \rho \rangle_\rho$ ➔ $\hat{S} = -\sum_\mu \log p_\mu \, |\phi_\mu\rangle\langle\phi_\mu|$

$E = \langle \hat{H} \rangle_\rho$ ➔ $\hat{H} = \sum_i E_i \, |i\rangle\langle i|$

Eigenstate of ρ

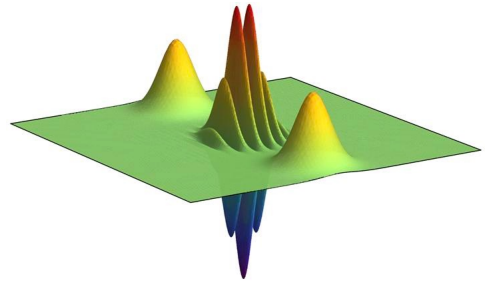
Energy eigenstate

$\boldsymbol{\Sigma = \Delta S - \beta \Delta E}$

but $\hat{S}$ and $\hat{H}$ may not commute in QM!

(c.f.) Negativity in the Wigner function

$$W(x,p) = \frac{1}{\pi\hbar}\int_{-\infty}^{\infty} \psi^*(x+y)\,\psi^*(x-y)e^{\frac{2ipy}{\hbar}}dy$$



✓ **Incompatible observables cannot be simultaneously measured ➔ $P_\rightarrow(\Sigma)$ is not well defined classically**

✓ **Possible solution: Introducing a quasi-probability distribution (allowing negative probabilities)**

- Does this quasi-probability of entropy production also satisfy the fluctuation theorem?

Yes! $$\frac{P_\rightarrow(\Sigma)}{P_\leftarrow(-\Sigma)} = e^{\Sigma}$$

[HK and M. Kim, PRX **9**, 031029 (2019)]

Even if $P_\rightarrow(\Sigma)$ can be negative
(in which case $P_\leftarrow(-\Sigma)$ also becomes negative)

Experimental realization of QFT

- **How do we obtain the quasi-probability in experiments?**

$S = \langle -\log\rho \rangle_\rho$ ➔ $\hat{S} = -\sum_\mu \log p_\mu \, |\phi_\mu\rangle\langle\phi_\mu|$

$E = \langle \hat{H} \rangle_\rho$ ➔ $\hat{H} = \sum_i E_i \, |i\rangle\langle i|$

Eigenstate of ρ

Energy eigenstate

$\boldsymbol{\Sigma = \Delta S - \beta \Delta E}$

➔ Perform POVMs before and after the quantum channel

ρ — $\{M_m\}$ — $\mathcal{N}$ — $\{M'_{m'}\}$ → $P(m,m') = \mathrm{Tr}\left[M'_{m'}\mathcal{N}\left(M_m \rho M_m^\dagger\right)M'^\dagger_{m'}\right]$

➔ We can find $\{M_m\}$, $\{M'_{m'}\}$, and some complex coefficients $\alpha_{mm'}$ such that

$$\boldsymbol{P_\rightarrow(\Sigma) = \sum_{m,m'} \alpha_{mm'} P(m,m')}$$ (Classical post-processing)

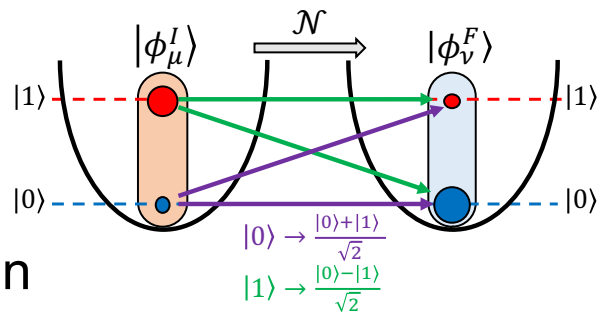
For more detail: [PRX **9**, 031029 (2019) & arXiv:2207.06106]

- **Main ingredients for testing quantum fluctuation theorems**

✓ Preparation of superposition state

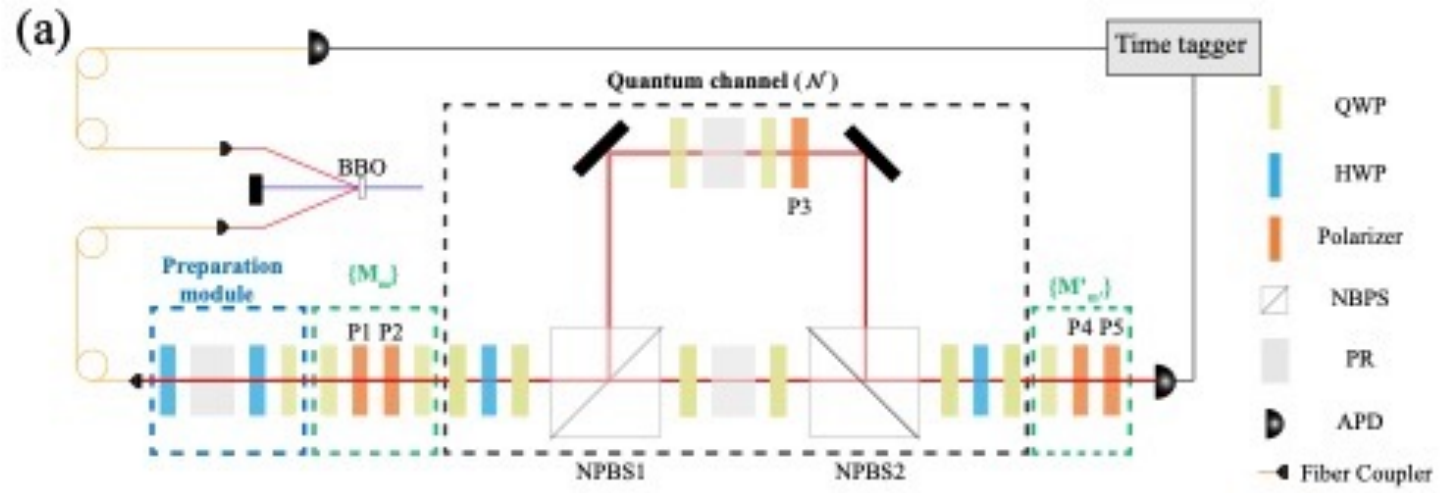
✓ Quantum channel inducing coherence

✓ POVM measurements to construct the quasi-probability of entropy production



Experimental realization of QFT

- **Experimental setup (state preparation)**



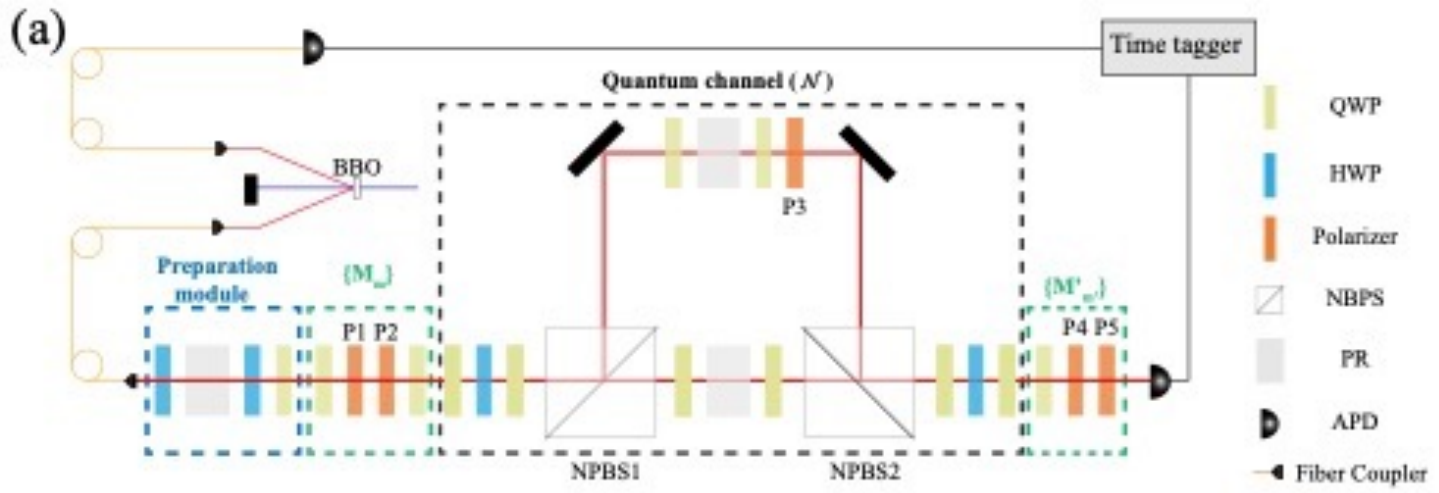
- We use a polarization degree of freedom: $|0\rangle$ ➔ Horizontal polarization, $|1\rangle$ ➔ Vertical polarization

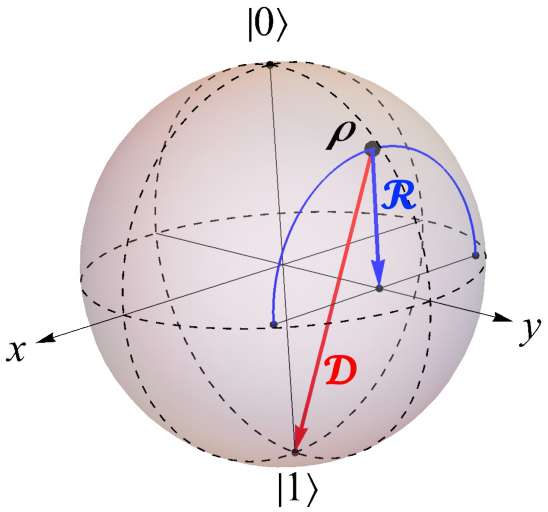
- Initial state: $\rho^I = \sum_{\mu=0,1} p_\mu^I |\phi_\mu^I\rangle\langle\phi_\mu^I|$
  with $p_0^I = \frac{4}{5}$, $p_1^I = \frac{1}{5}$ and $|\phi_0^I\rangle = \cos\left(\frac{\pi}{6}\right)|0\rangle + i\sin\left(\frac{\pi}{6}\right)|1\rangle$, $|\phi_1^I\rangle = \sin\left(\frac{\pi}{6}\right)|0\rangle - i\cos\left(\frac{\pi}{6}\right)|1\rangle$

- Final state: $\rho^F = \mathcal{N}(\rho^I) = \sum_{\nu=0,1} p_\nu^F |\phi_\nu^F\rangle\langle\phi_\nu^F|$

Experimental realization of QFT

- **Experimental setup (implementing the quantum channel)**

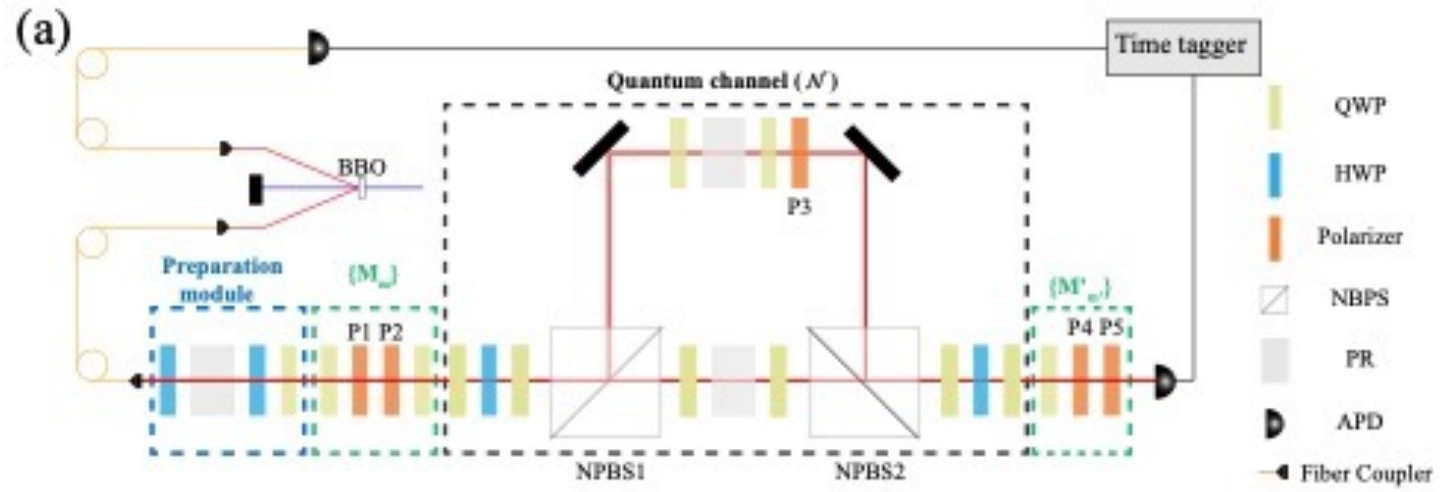


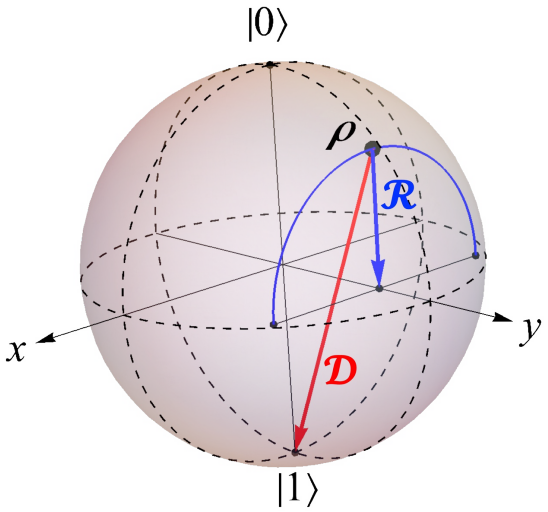


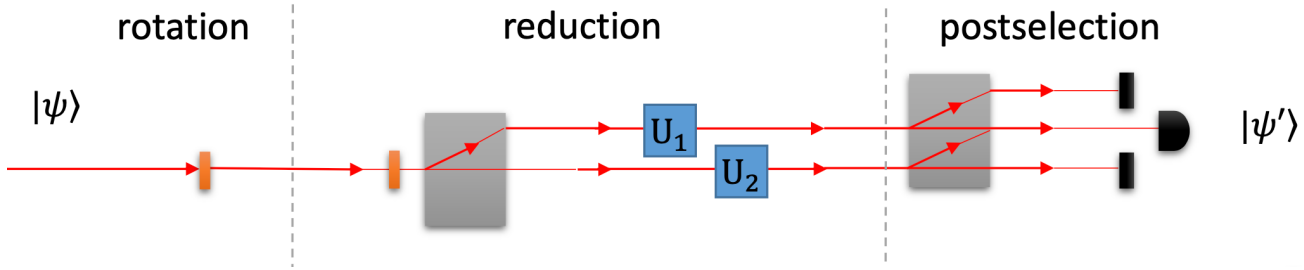
- (Noisy) quantum channel: $\mathcal{N}(\rho) = p\rho + (1-p)[(1-s)\mathcal{R}(\rho) + s\mathcal{D}(\rho)]$
- Stationary state: $\gamma = \left(\frac{1-s}{2}\right)|0\rangle\langle 0| + \left(\frac{1+s}{2}\right)|1\rangle\langle 1| = \frac{1}{Z}e^{-\beta\sigma_z}$ $(\mathcal{N}(\gamma) = \gamma)$
- **The backward process is the same as the forward process**
  (a.k.a. detailed balance condition)

Experimental realization of QFT

- **Experimental setup (implementing the quantum channel)**

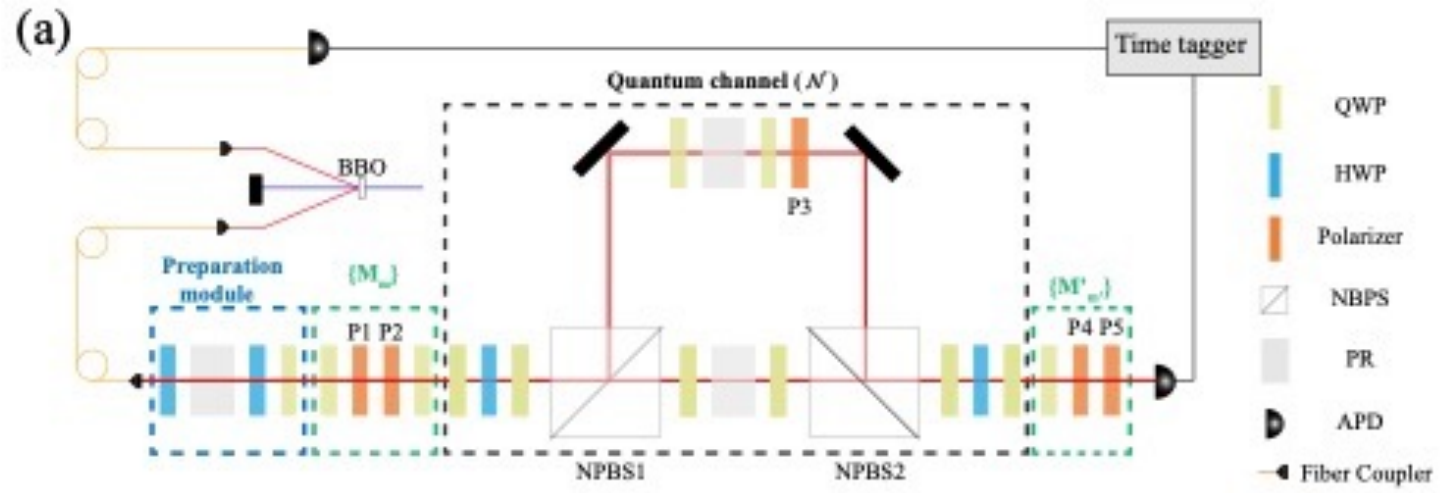






Experimental realization of QFT

- **Experimental setup (POVM measurements)**



✓ To get $P_{\rightarrow}(\Sigma)$, 8 POVM elements are needed at each time

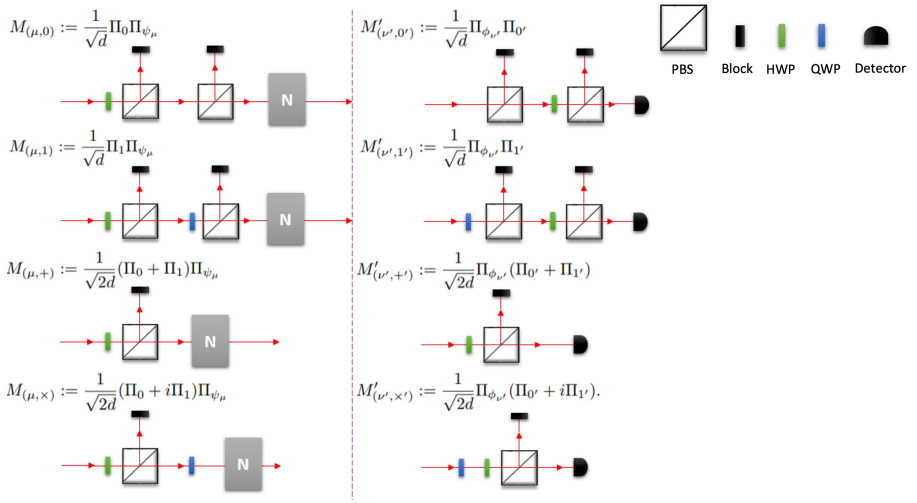
$$M_{(\mu,0)} = \frac{\Pi_0 \Pi_{\phi_\mu}}{\sqrt{2}}$$

$$M_{(\mu,1)} = \frac{\Pi_1 \Pi_{\phi_\mu}}{\sqrt{2}}$$

$$M_{(\mu,+)} = \frac{(\Pi_0 + \Pi_1)\Pi_{\phi_\mu}}{2}$$

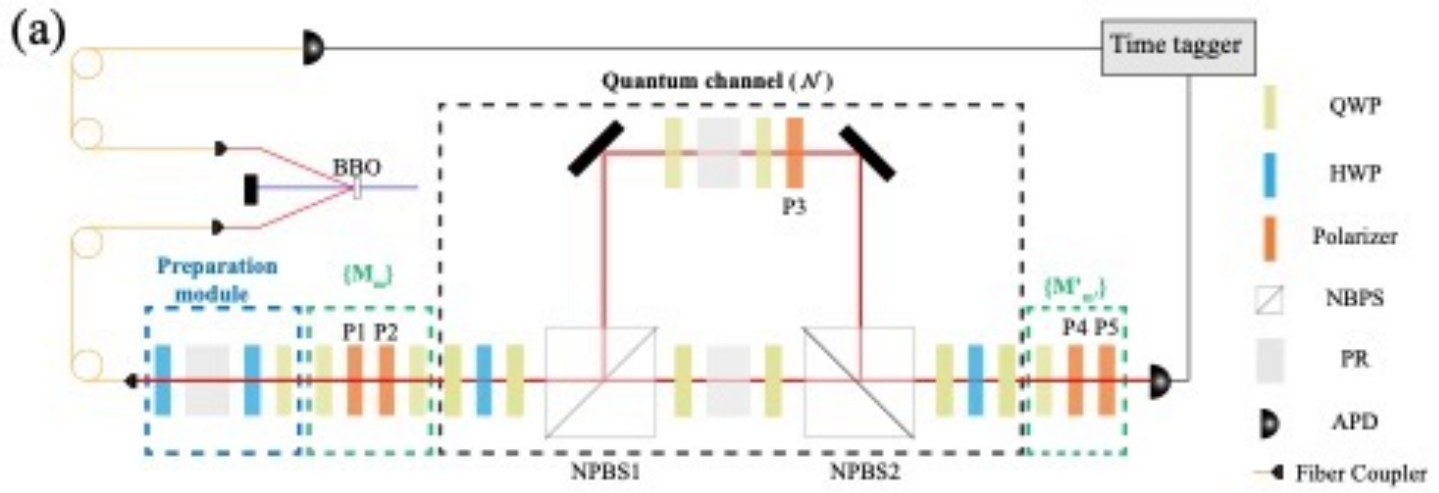
$$M_{(\mu,\times)} = \frac{(\Pi_0 + i\Pi_1)\Pi_{\phi_\mu}}{2}$$

* Π_{ϕ_μ}: projection to the eigenstate of ρ^I



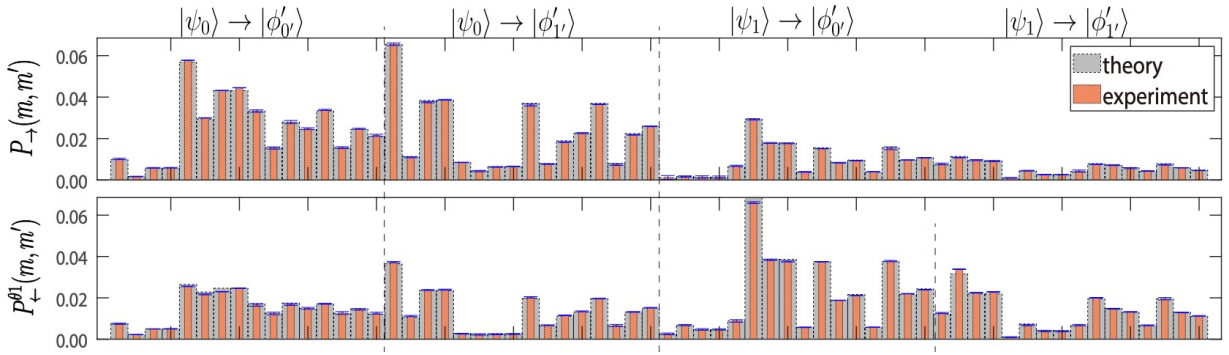
Experimental results

- **Reconstructing the quasi-probability distribution**



ρ^I for the forw

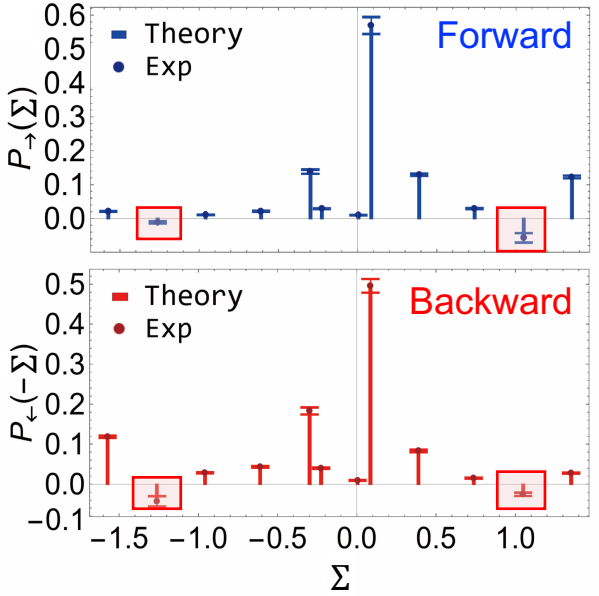
$\rho^F = \mathcal{N}(\rho^I)$ fo. the backward process



Measurement outcomes (m, m')

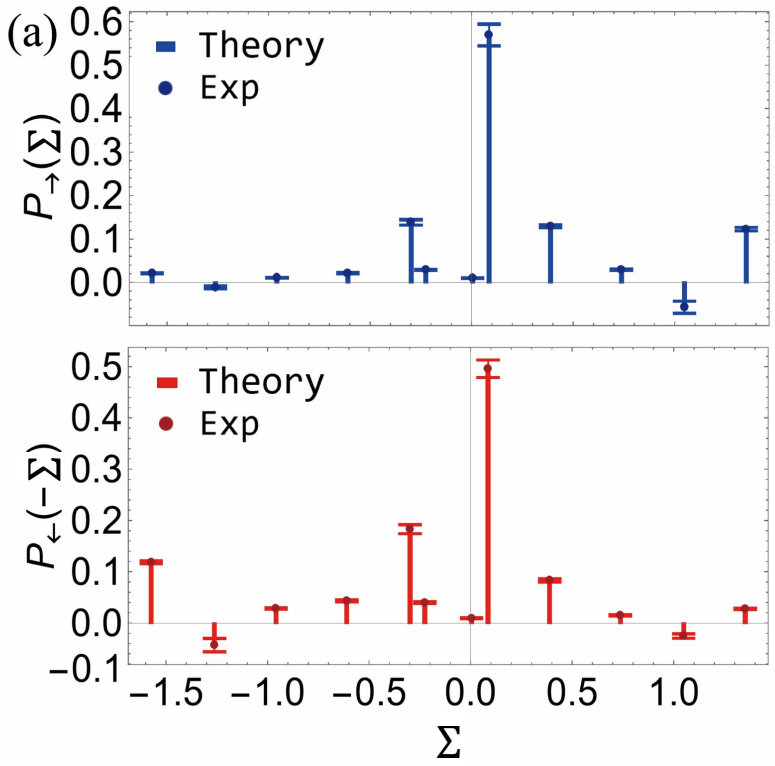
Classical post-processing

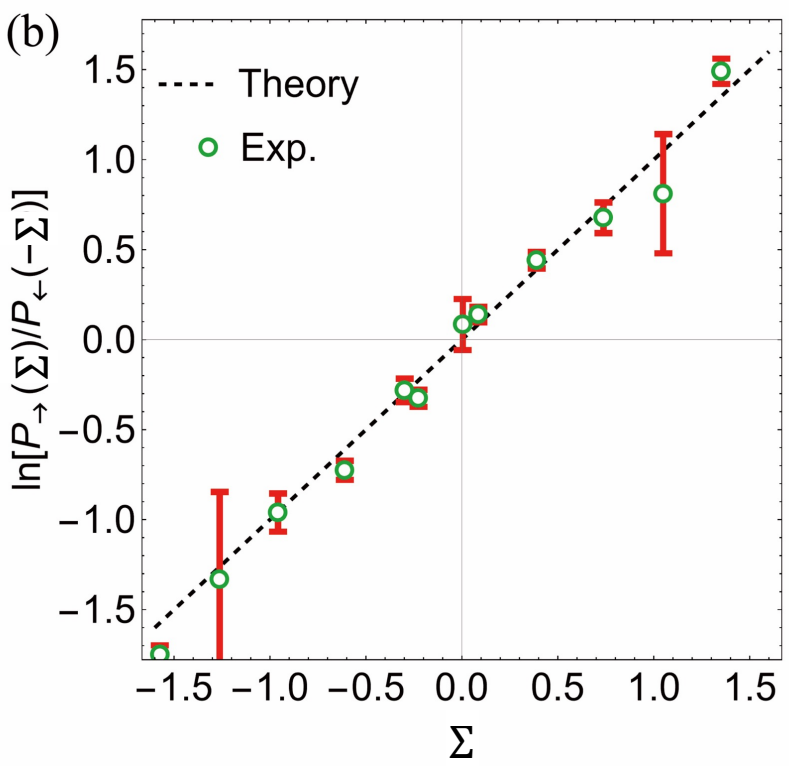
$$P_{\to}(\Sigma) = \sum_{m,m'} \alpha_{mm'} P(m,m')$$

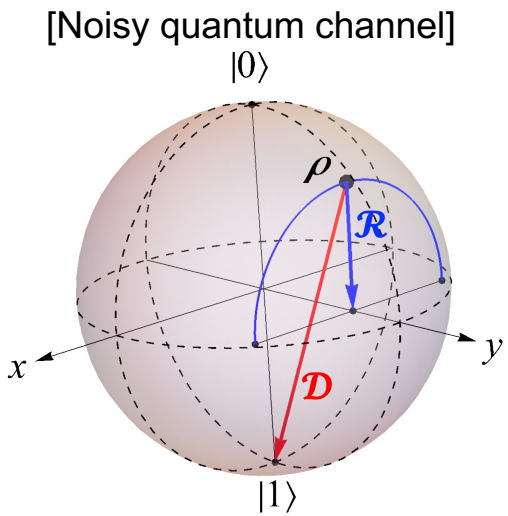


Experimental results

- **Verification of quantum fluctuation theorem**







$\langle e^{-\Sigma} \rangle_{\mathbf{exp}} = \mathbf{0.99 \pm 0.02}$

Integral fluctuation theorem (Jarzynski equality)

$\langle e^{-\Sigma} \rangle = \sum_{\Sigma} P_{\rightarrow}(\Sigma)\, e^{-\Sigma} = \sum_{\Sigma} P_{\leftarrow}(-\Sigma) = 1$

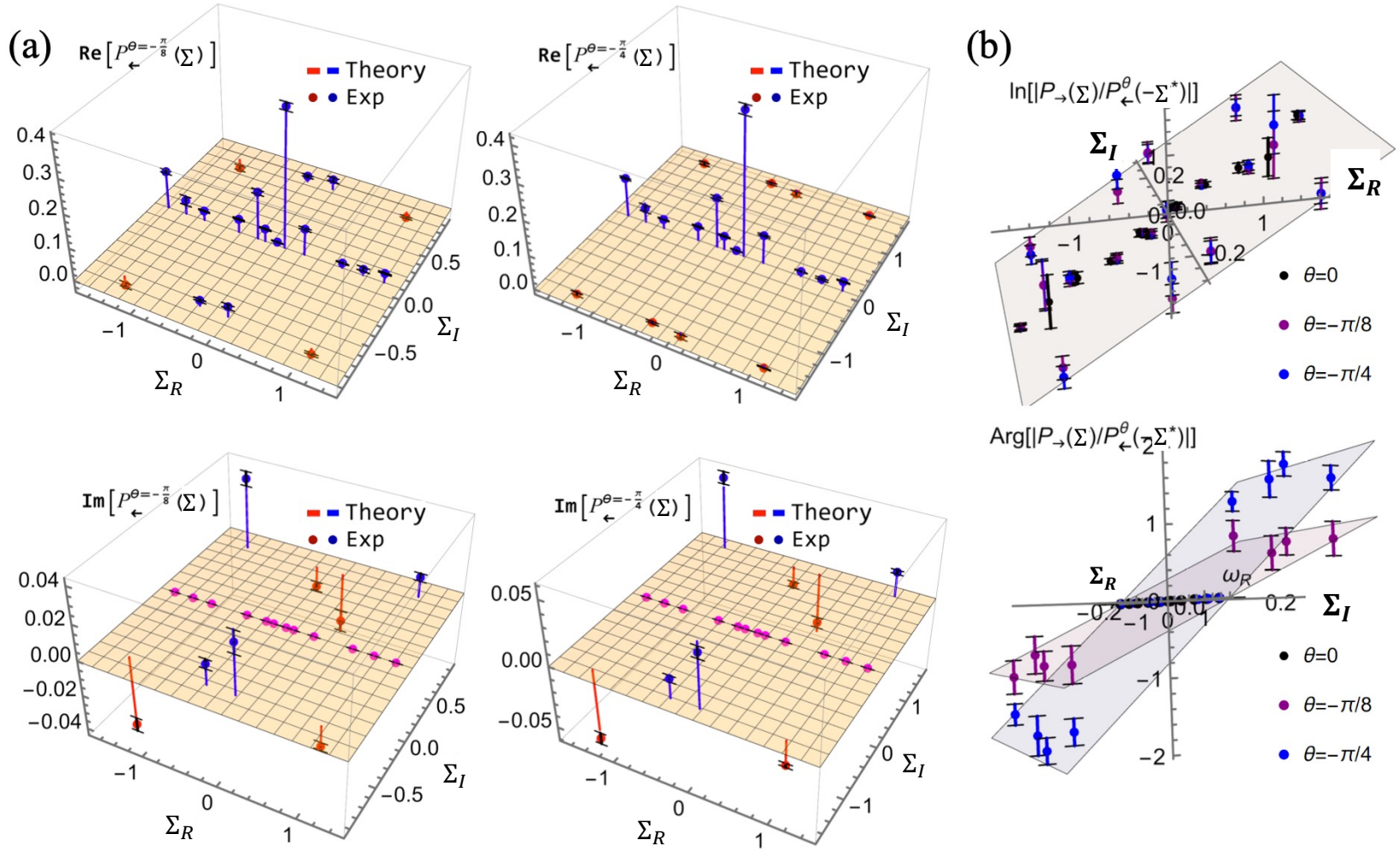
$\langle e^{-\Sigma} \rangle_{\mathbf{exp}} = \mathbf{0.99 \pm 0.02}$

$$\log\left[\frac{P_{\rightarrow}(\Sigma)}{P_{\leftarrow}(-\Sigma)}\right] = \Sigma \Leftrightarrow \frac{P_{\rightarrow}(\Sigma)}{P_{\leftarrow}(-\Sigma)} = e^{\Sigma}$$

Fluctuation theorem also holds in the quantum regime!

But this is not the whole story…

- **Entropy production can be even complex-valued! ➔ $\boldsymbol{\Sigma = \Sigma_R + i\Sigma_I}$**



$$\frac{P_{\rightarrow}(\Sigma)}{P^{\theta}_{\leftarrow}(-\Sigma^*)} = e^{\Sigma_R - 2i\theta\Sigma_I}$$

No classical counterpart
(purely quantum effect)

For more detail: HK & M. Kim, PRX **9**, 031029 (2019) & Jie Xie *et al.* (in preparation)

Quantum correlation function and quasi-probability

- Quantum correlation function

Suppose that we want to obtain the correlation between observables $\boldsymbol{A} = \left(A^{(1)}, A^{(2)}, \cdots, A^{(N)}\right)$ at multiple time points $\boldsymbol{t} = (t_1, t_2, \cdots, t_N)$

Then, a general form of quantum correlation function is given as

$$\boldsymbol{C_A(t)} = \mathrm{Tr}\left[\rho A^{(1)}(t_1)A^{(2)}(t_2)\cdots A^{(N)}(t_N)\right]$$

where $A(t) = U_{0\to t}^{\dagger} A U_{0\to t}$ is an operator in the Heisenberg picture.

- ✓ $A_{tot}(\boldsymbol{t}) \coloneqq A^{(1)}(t_1)A^{(2)}(t_2)\cdots A^{(N)}(t_N)$ is in general non-Hermitian operator
- ✓ $\boldsymbol{C_A(t)}$ is complex-valued ➔ Cannot be directly obtained from a single observable
- ✓ One way to evaluate this: $\boldsymbol{C_A(t)} = \mathrm{Tr}\left[\rho \frac{\left(A_{tot}(t)+A_{tot}^{\dagger}(t)\right)}{2}\right] + i\mathrm{Tr}\left[\rho \frac{\left(A_{tot}(t)-A_{tot}^{\dagger}(t)\right)}{2i}\right]$

Measurement induced back-action

- Some indirect approaches

✓ Separately measure the real and imaginary parts: $\boldsymbol{C_A(t)} = \mathrm{Tr}\left[\rho \frac{\left(A_{tot}(t)+A_{tot}^{\dagger}(t)\right)}{2}\right] + i\mathrm{Tr}\left[\rho \frac{\left(A_{tot}(t)-A_{tot}^{\dagger}(t)\right)}{2i}\right]$

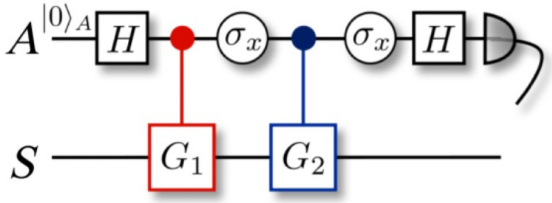
If the system dynamics changes observables should be constructed differently

✓ Weak measurement: **Not entirely free from measurement-disturbance relation**

Some ways to detour: 1) combining various types of measurements PRA 76, 012119 (2007)
2) Using multiple copies: PRL 118, 070601 (2017)

✓ Quantum circuit

[Characteristic function
- PRL 110, 230602 (2013)]

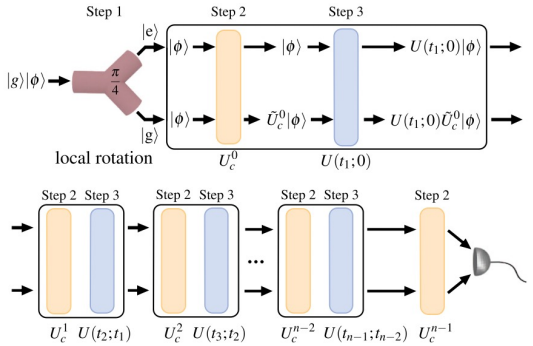


$$\chi(u,v) = \mathrm{Tr}[U_{t_1\to t_2}\rho e^{iAu}U_{t_1\to t_2}^{\dagger}e^{-iAv}]$$

$$\downarrow$$

$$Q_{i_1 i_2}(t_1,t_2)$$

[Multi-point Hadamard test - PRL 113, 020505 (2014)]



$$|\phi\rangle\left(\frac{|e\rangle+|g\rangle}{\sqrt{2}}\right) \to \frac{|\phi\rangle|e\rangle+Z|\phi\rangle|g\rangle}{\sqrt{2}}$$

$$\to \frac{U|\phi\rangle|e\rangle+UZ|\phi\rangle|g\rangle}{\sqrt{2}}$$

$$\to \frac{U|\phi\rangle|e\rangle+ZUZ|\phi\rangle|g\rangle}{\sqrt{2}}$$

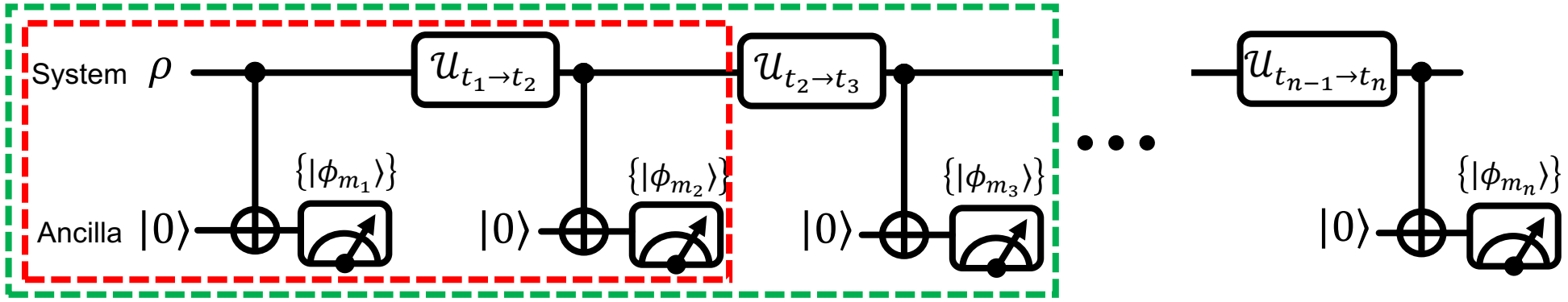
$$\to \frac{1}{2}\left((U|\phi\rangle+ZUZ|\phi\rangle)|e\rangle+(U|\phi\rangle-ZUZ|\phi\rangle)|g\rangle\right)$$

$$\rightarrow P_e = (1+\mathrm{Re}[C_{ZZ}(t_1,t_2)])/2$$

Requires long time coherence between the system and ancilla states

Back-action free extraction of quantum statistics

- The protocol:

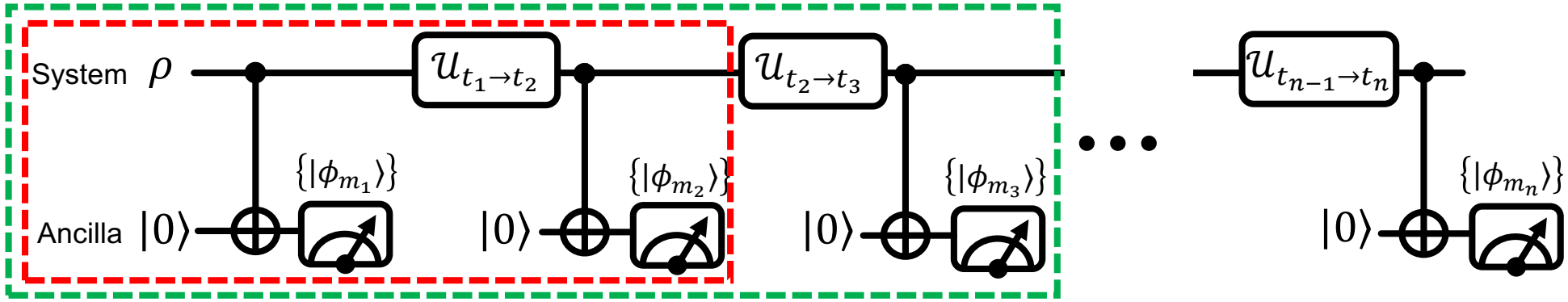


$\mathcal{P}_{m_1,m_2,\cdots,m_N}(t_1,t_2,\cdots t_N)$ ➔ $C_{\boldsymbol{A}}(\boldsymbol{t}) = \mathbb{E}[\gamma_{\boldsymbol{m}}(\boldsymbol{A})]$, $\mathcal{Q}_{i_1 i_2 \cdots i_N}(\boldsymbol{t}) = \mathbb{E}[\gamma_{\boldsymbol{m}}(\boldsymbol{\Pi_i})]$

1. Prepare the system state ρ
2. Ancilla-assisted measurement
   a. Initialize the ancilla state to $|0\rangle$
   b. Apply interaction between the system and ancilla states
   c. Measure the ancilla state with respect to $\{|\phi_m\rangle\}$
3. Let the system evolve
4. Repeat 2-3 and record the measurement trajectory $\boldsymbol{m} = (m_1, m_2, \cdots, m_N)$
5. Collect many trajectories of $\boldsymbol{m}$ by repeating 1-5
6. By ensemble averaging the trajectory data with a proper weight γ_m, evaluate the quantum statistics

Back-action free extraction of quantum statistics

- The protocol:



$\mathcal{P}_{m_1,m_2,\cdots,m_N}(t_1,t_2,\cdots t_N)$ ➔ $C_{\boldsymbol{A}}(\boldsymbol{t}) = \mathbb{E}[\gamma_{\boldsymbol{m}}(\boldsymbol{A})]$, $\mathcal{Q}_{i_1 i_2 \cdots i_N}(\boldsymbol{t}) = \mathbb{E}[\gamma_{\boldsymbol{m}}(\boldsymbol{\Pi_i})]$

Pros:

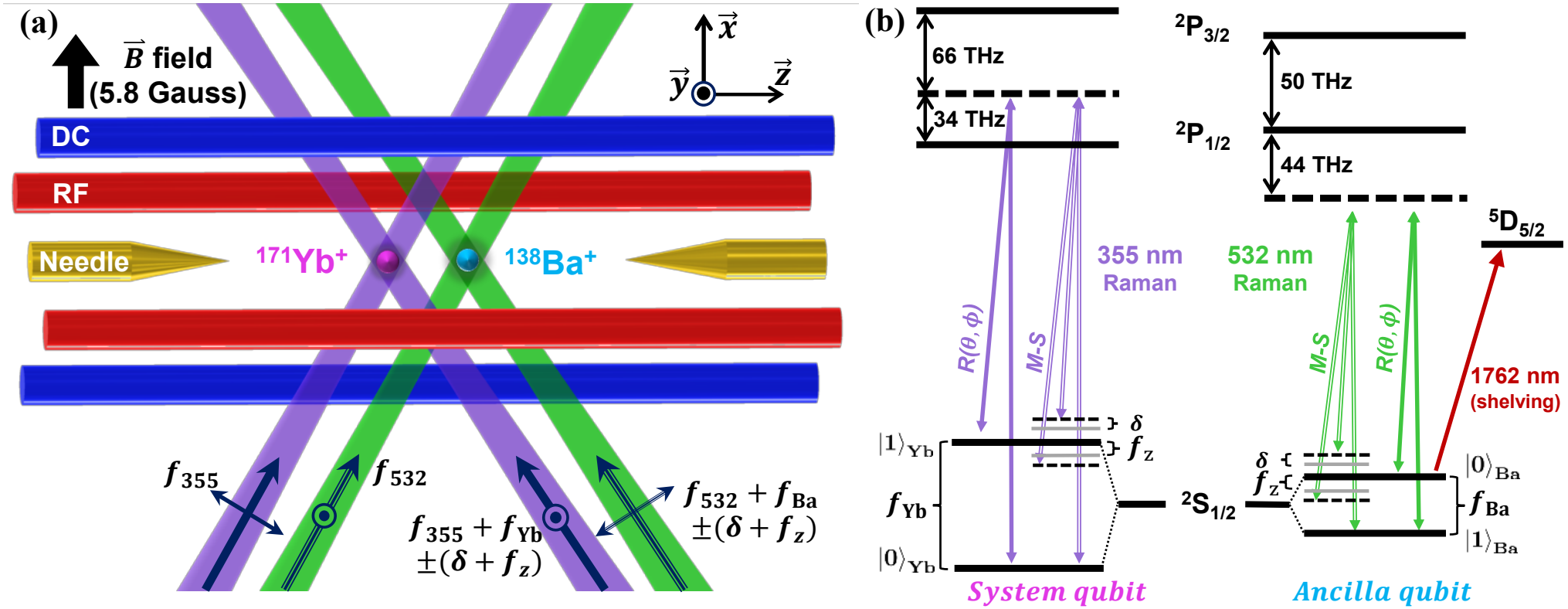
1) Only require **a single-copy state** preparation at the same time
2) **Short coherence time** between system-ancilla is enough
3) Measurement protocol is **independent of the system dynamics**

Cons:

1) **More samples** are needed to get an accurate result ← (# of Samples) $\propto (\max|\gamma_{\boldsymbol{m}}|)^2$
   (c.f. measurement-disturbance trade-off)
2) Ancilla states should be initialized and measured **repeatedly**

Experimental realization

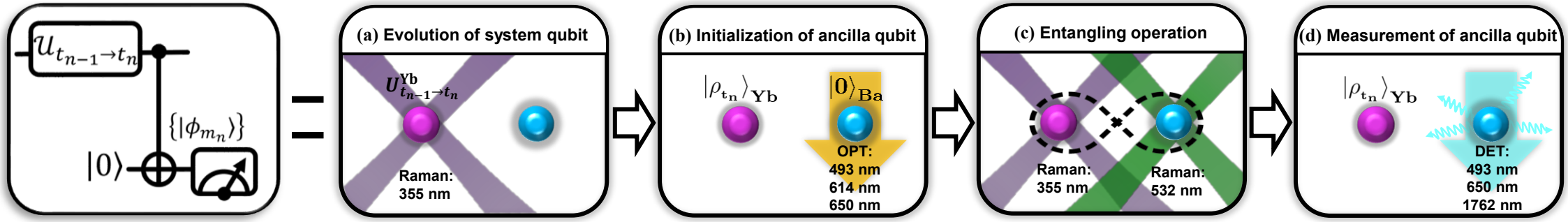
- Dual species (Yb-Ba) trapped ion system



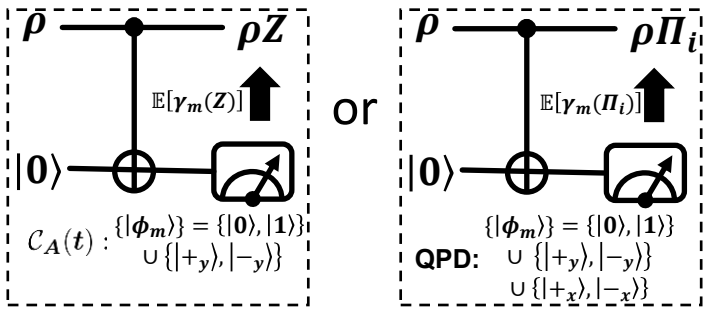
✓ Different frequencies are used to control two different atoms ➔ **Minimal influence**

Experimental realization

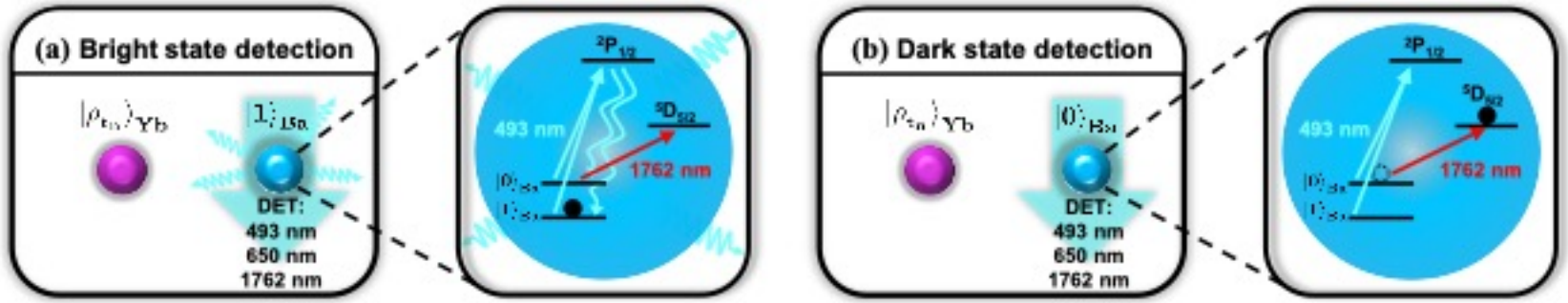
- Realizing ancilla-assisted measurement protocol



✓ Post-selection of the dark state (to minimize heat)



or



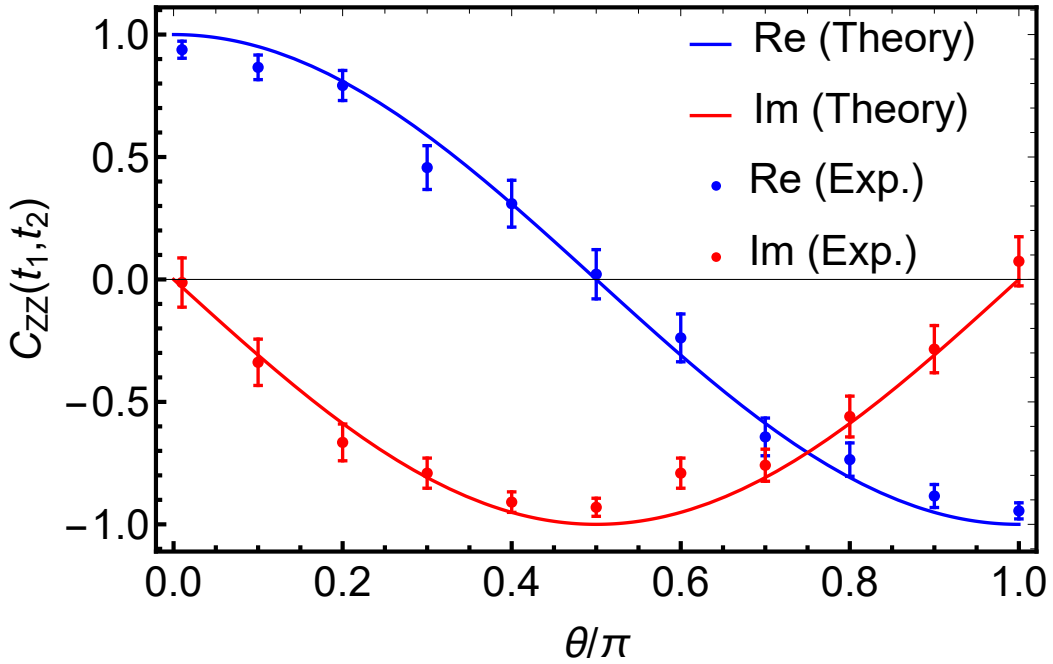
Experimental results – Two-point quantum statistics

- Two-point quantum statistics

✓ **System dynamics:** $U_{t_1 \to t_2} = R_x(\theta)$

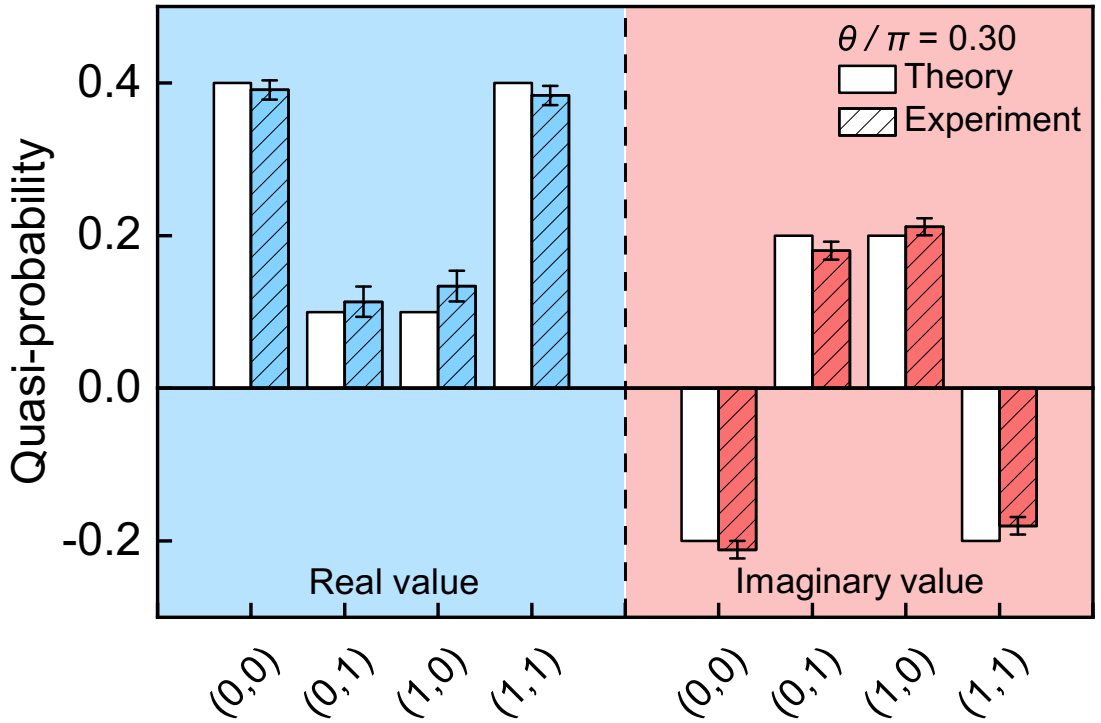
✓ Correlation function

$$C_{ZZ}(t_1, t_2) = \mathrm{Tr}[\rho Z(t_1) Z(t_2)]$$
$$= \mathrm{Tr}\left[U_{t_1 \to t_2} \rho Z U_{t_1 \to t_2}^{\dagger} Z\right]$$



✓ Quasi-probability

$$Q_{i_1,i_2}(t_1, t_2) = \mathrm{Tr}\left[\rho \Pi_{i_1}(t_1) \Pi_{i_2}(t_2)\right]$$
$$= \mathrm{Tr}\left[U_{t_1 \to t_2} \rho \Pi_{i_1} U_{t_1 \to t_2}^{\dagger} \Pi_{i_2}\right]$$



Experimental results – Three-point quantum statistics

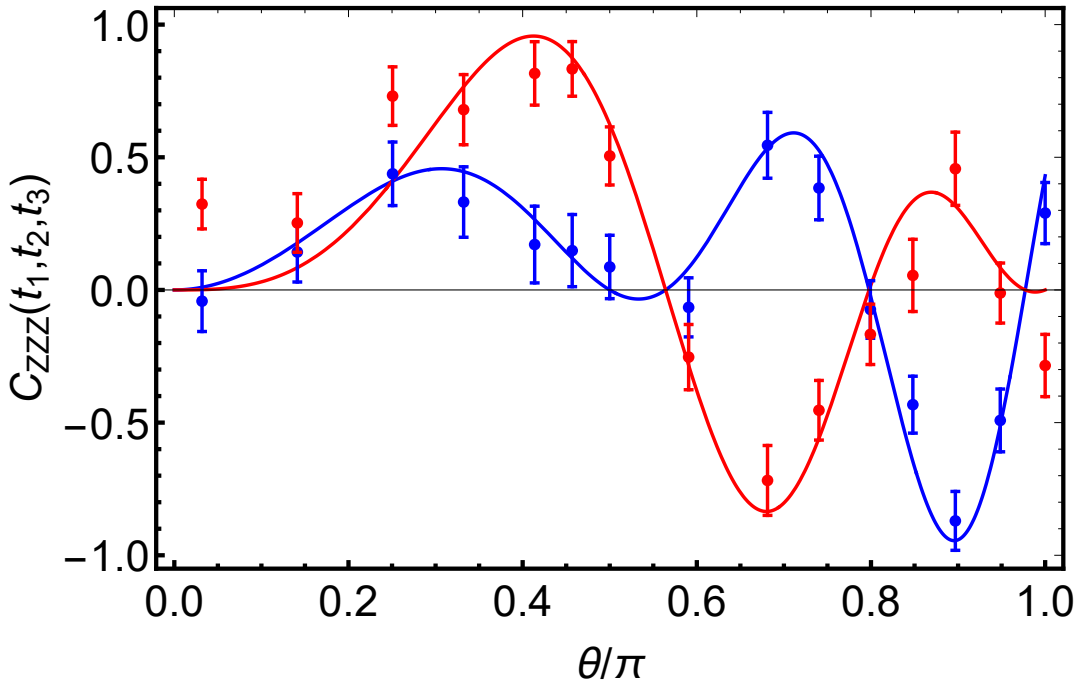
- Three-point quantum statistics

✓ **System dynamics:** $U_{t_1 \to t_2} = R_x(\theta)$

$U_{t_2 \to t_3} = R_y(\theta^2)$

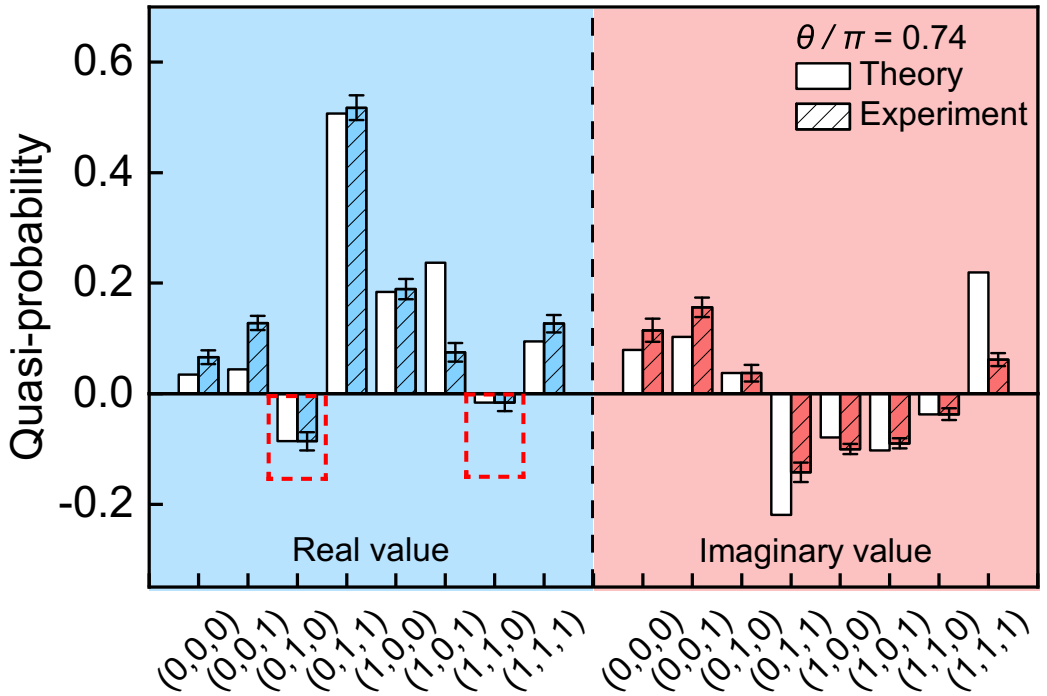
✓ Correlation function

$$C_{ZZZ}(t_1, t_2, t_3) = \mathrm{Tr}[\rho Z(t_1) Z(t_2) Z(t_3)]$$
$$= \mathrm{Tr}\left[U_{t_2 \to t_3} U_{t_1 \to t_2} \rho Z U_{t_1 \to t_2}^{\dagger} Z U_{t_2 \to t_3}^{\dagger} Z\right]$$



✓ Quasi-probability

$$Q_{i_1,i_2,i_3}(t_1, t_2, t_3) = \mathrm{Tr}\left[\rho \Pi_{i_1}(t_1) \Pi_{i_2}(t_2) \Pi_{i_3}(t_3)\right]$$
$$= \mathrm{Tr}\left[U_{t_2 \to t_3} U_{t_1 \to t_2} \rho \Pi_{i_1} U_{t_1 \to t_2}^{\dagger} \Pi_{i_2} U_{t_2 \to t_3}^{\dagger} \Pi_{i_3}\right]$$

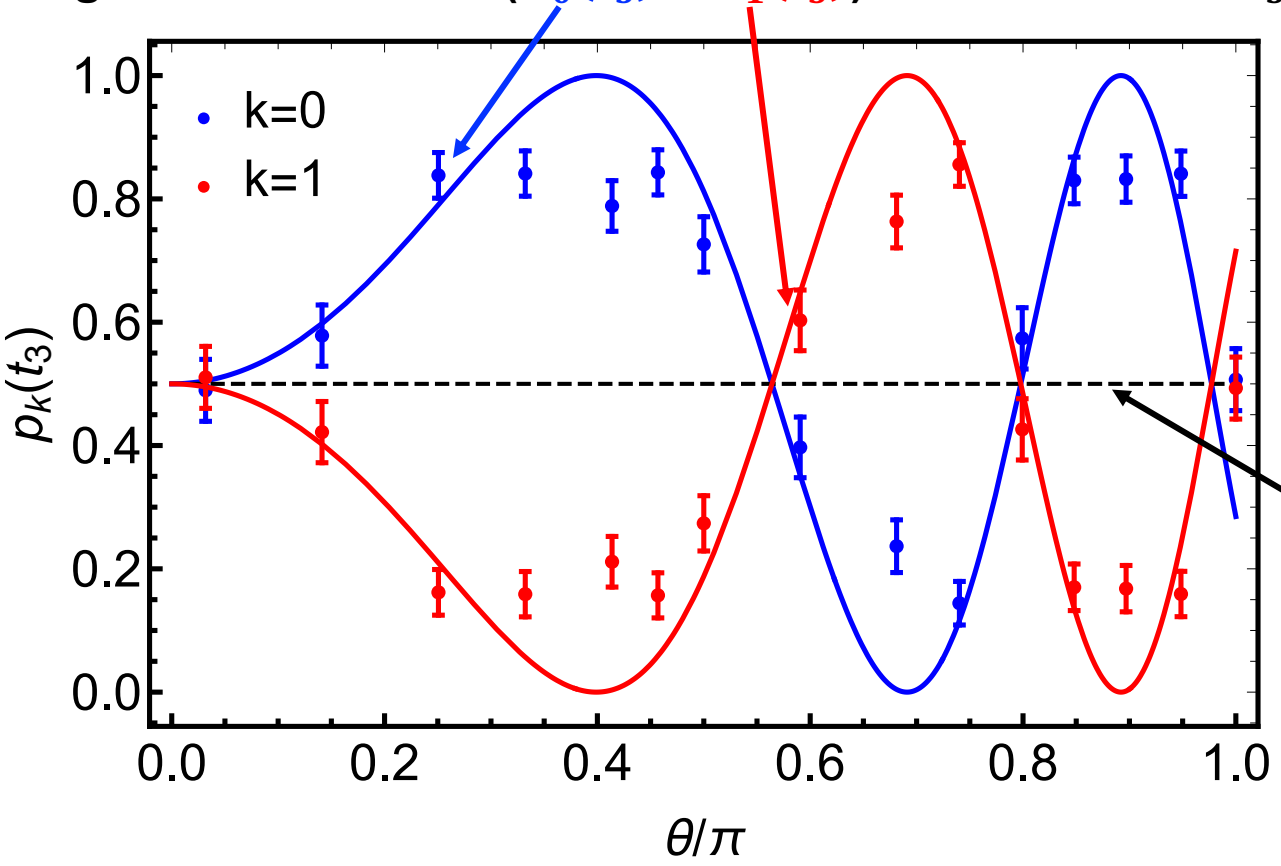


Experimental results – Marginal distributions

$$\boldsymbol{Q}_{i_1 i_2 \cdots i_N}(\boldsymbol{t}) = \mathrm{Tr}\left[\rho \Pi_{i_1}^{(1)}(t_1)\Pi_{i_2}^{(2)}(t_2)\cdots\Pi_{i_N}^{(N)}(t_N)\right]$$

✓ $\sum_{i_1,i_2,\cdots,i_{N-1}} \boldsymbol{Q}_{i_1 i_2 \cdots i_N}(\boldsymbol{t}) = \mathrm{Tr}\left[\rho \Pi_{i_N}^{(N)}(t_N)\right]$: Correct marginal distribution (at each point) ($\because \sum_i \boldsymbol{\Pi_i} = \mathbb{I}$)

Marginal distributions ($P_0(t_3)$ & $P_1(t_3)$) at the final time t_3



If the projective measurement is performed at t_1

$|+\rangle \rightarrow \frac{|0\rangle\langle 0| + |1\rangle\langle 1|}{2} = \frac{\mathbb{I}}{2}$

$U\left(\frac{\mathbb{I}}{2}\right)U^\dagger = \frac{\mathbb{I}}{2}$ for any unitary evolution

$\therefore$ Population is always balanced

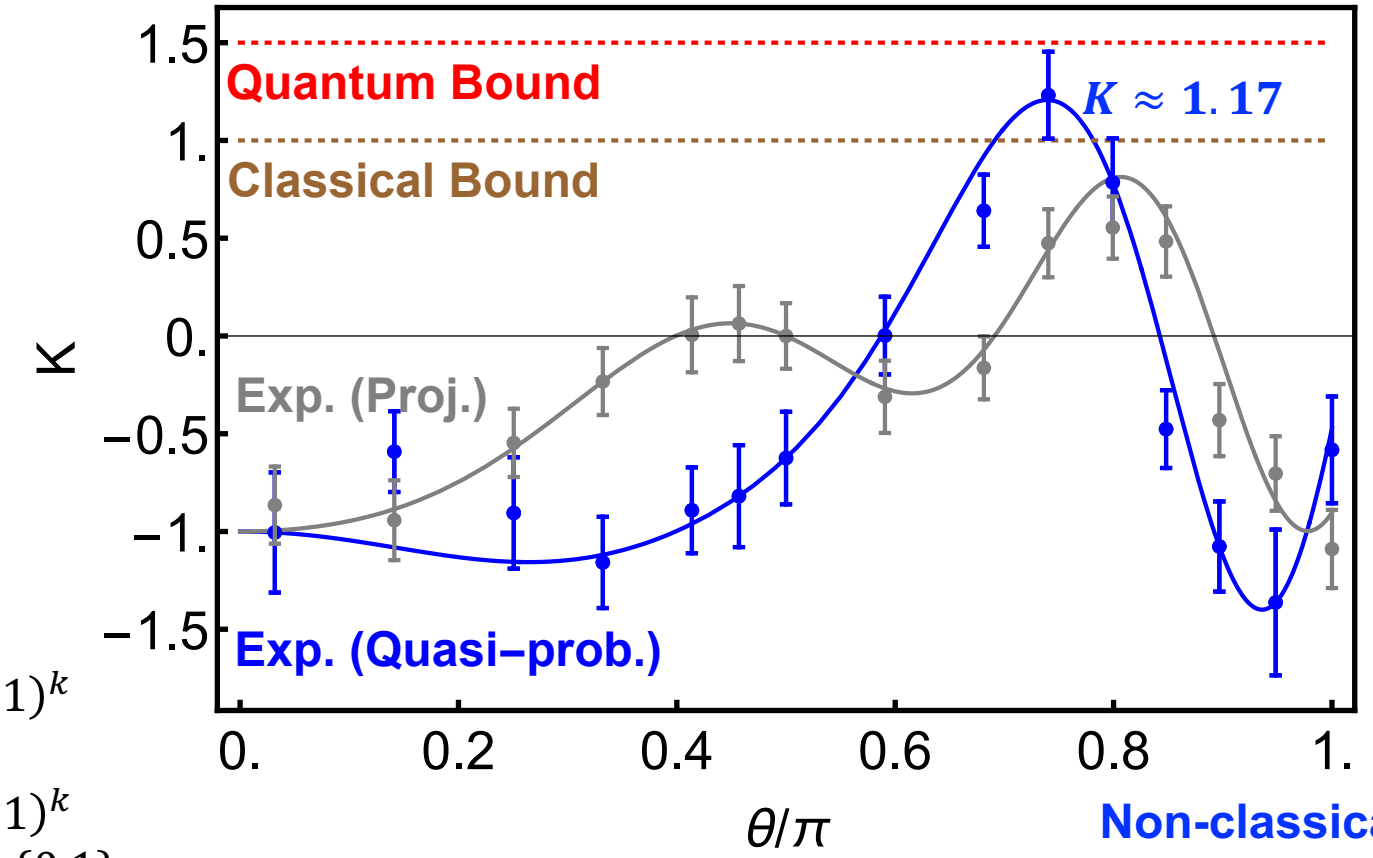
The QPD preserves the marginal distribution!

Experimental results – Leggett-Garg inequality

✓ Leggett-Garg inequality (1985)

$K = \langle E(t_1)E(t_2)\rangle + \langle E(t_2)E(t_3)\rangle - \langle E(t_1)E(t_3)\rangle \leq 1$ (for classical joint probability distributions)

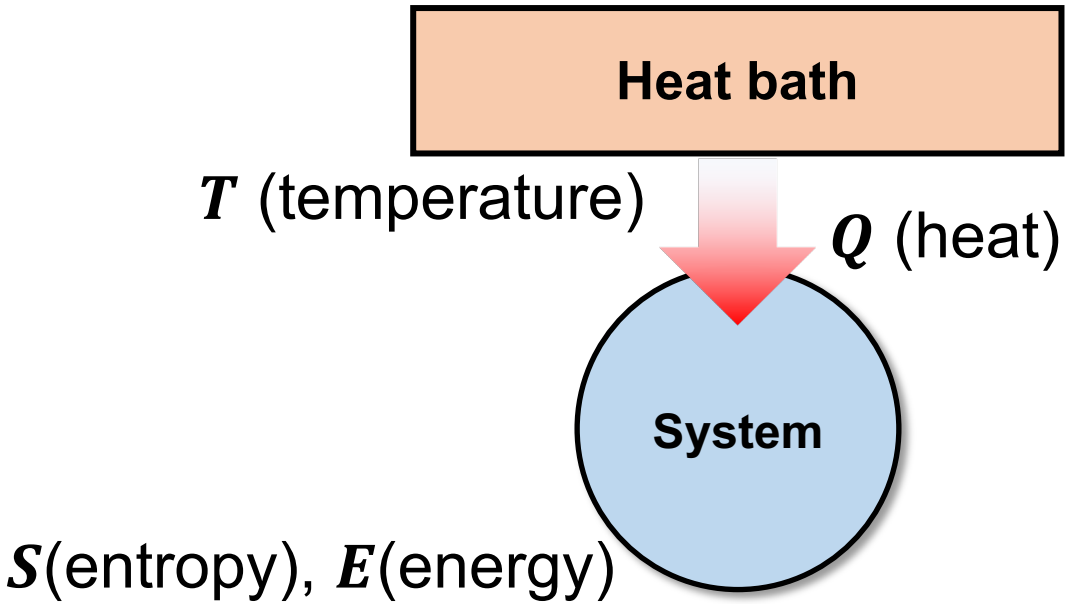
Coherent evolution of the system can reach $K > 1$



$E(t_1) = (-1)^k$
$E(t_2) = 1$
$E(t_3) = (-1)^k$
$k \in \{0,1\}$

Non-classicality of the QPD is verified!

Thermodynamic potential



The second law (classical, formal statement)

$$\Delta S \geq \frac{Q}{T} \qquad \delta Q = T dS$$

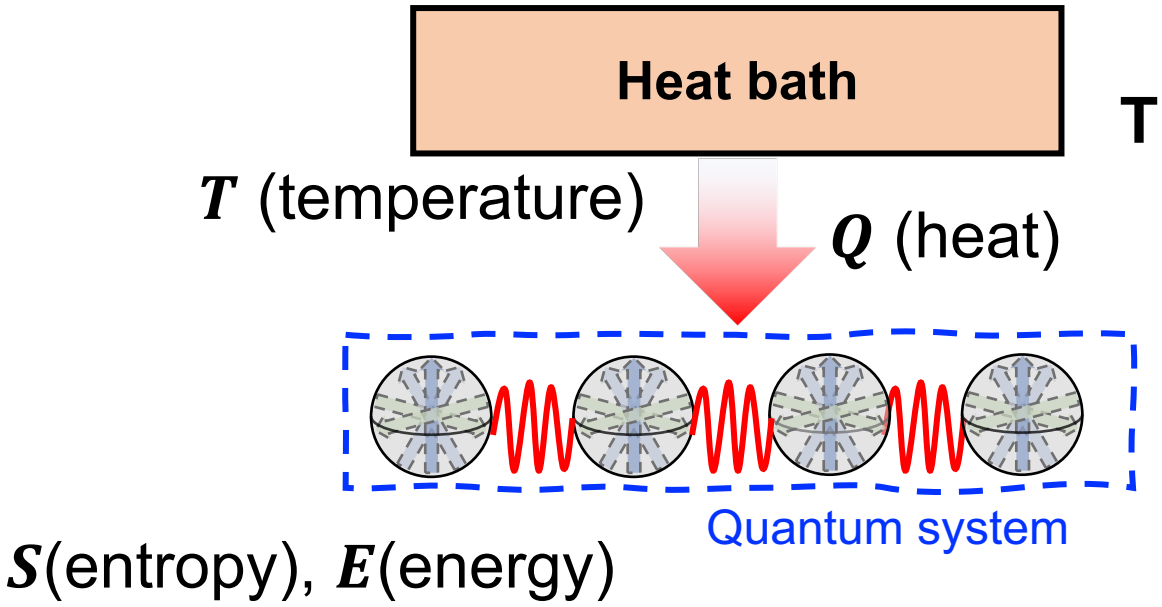
(Equality holds only for a reversible process)

$$\Rightarrow T\Delta S \geq \Delta E - W \quad (Q + W = \Delta E)$$

$$\Rightarrow W \geq \Delta E - T\Delta S = \Delta F$$

- **(Helmholtz) free energy: $F = E - TS$**
  - ➔ Maximum amount of **work** that can be **extracted** from the system
  - ➔ Free energy is **minimized** when the system is **at equilibrium**

Thermodynamic potential



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- **(Helmholtz) free energy: $F = E - TS$**

  ➔ Maximum amount of **work** that can be **extracted** from the system

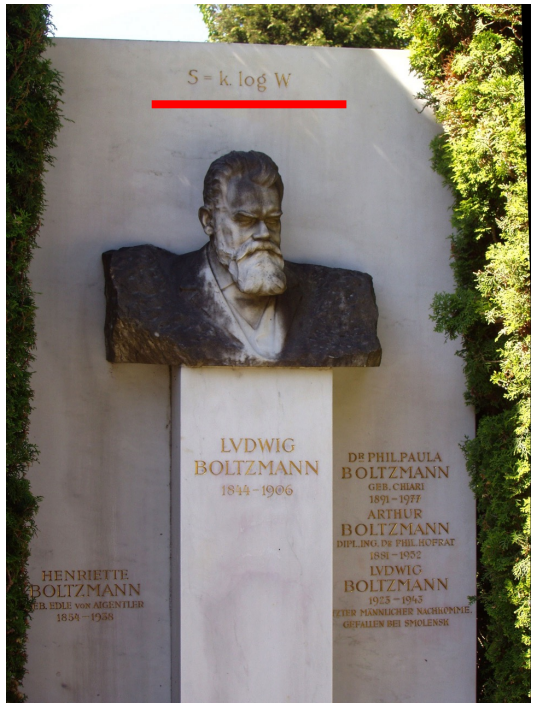
  ➔ Free energy is **minimized** when the system is **at equilibrium**

Can we define free energy for a quantum system?

[Nat. Commun. **4**, 2059 (2013); PRL **111**, 250404 (2013); PNAS **112**, 3275 (2015); Nat. Commun. **6**, 6383 (2015)]

Various definitions of entropy

Thermodynamic definition (by Boltzmann)



$S = k_B \log \Omega$

Ω: Number of microscopic states

Equal probability

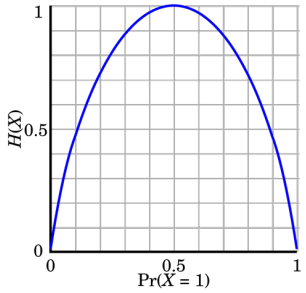
$\geq$

Information-theoretic definition (by Shannon)



Head: p Tail: $1\text{-}p$

…	1	1	0	1	0	1	0	0	…

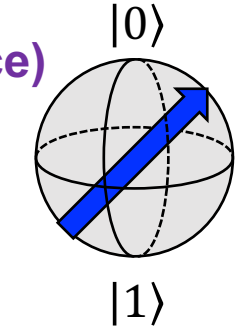


$$S(p) = -\sum_x p(x) \log p(x)$$

$p(x)$: Probability distribution over events/states

Diagonal state (without coherence)

$\geq$



Quantum Information (by von Neumann)

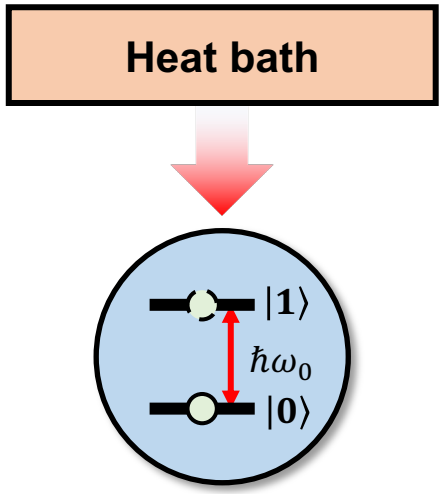
$$\rho = \begin{pmatrix} \rho_{00} & \rho_{01} \\ \rho_{10} & \rho_{11} \end{pmatrix} = V \begin{pmatrix} p & 0 \\ 0 & 1-p \end{pmatrix} V^\dagger$$

$S(\rho) = -\mathrm{Tr}[\rho \log \rho]$

ρ: Quantum density matrix

Quantum and classical entropy

- Major difference between quantum and classical system
  ➔ **Superposition principle**



- Consider an example of a two-level system

  ➔ At equilibrium, $P_{eq}(E) = \frac{1}{Z}e^{-\beta E} = \begin{cases} \frac{1}{1+e^{-\beta\hbar\omega_0}} & (E=0) \\ \frac{e^{-\beta\hbar\omega_0}}{1+e^{-\beta\hbar\omega_0}} & (E=\hbar\omega_0) \end{cases}$

  ➔ Classical (Shannon) entropy of the system: $S\left(P_{eq}(E)\right) = \beta\langle E\rangle_{eq} + \log Z = \frac{\beta\hbar\omega_0}{1+e^{\beta\hbar\omega_0}} + \log\left(1+e^{-\beta\hbar\omega_0}\right)$

- For a quantum state, $|\psi\rangle = \sqrt{P_{eq}(E_0)}|0\rangle + \sqrt{P_{eq}(E_1)}|1\rangle = \sqrt{p_0}|0\rangle + \sqrt{p_1}|1\rangle$

  ➔ **Energy distribution is the same** as the equilibrium distribution $P_{eq}(E)$ ➔ $\langle E\rangle_\psi = \langle E\rangle_{eq}$

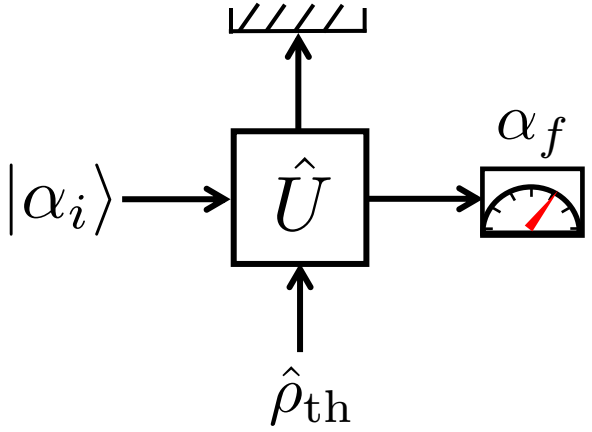
  ➔ However, quantum (von Neumann) entropy of the system: $\boldsymbol{S_Q = S(|\psi\rangle\langle\psi|) = 0 \le S\left(P_{eq}(E)\right) = S_{eq}}$

$$\boldsymbol{F_Q = \langle E\rangle_\psi - TS_Q \ge \langle E\rangle_{eq} - TS_{eq} = -\log Z = F_{cl}}$$

Quantum free energy can be larger

Quantum modification of microscopic reversibility

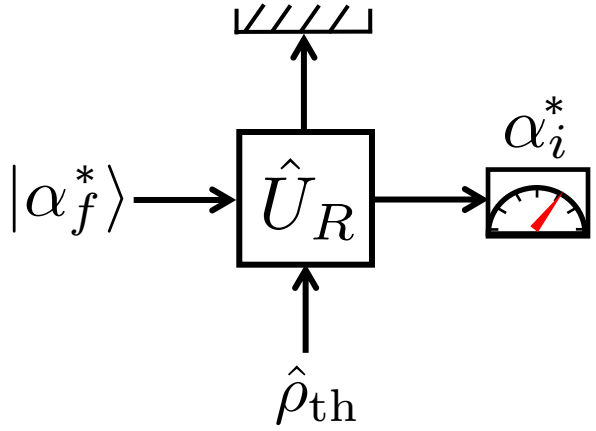
[Forward process]



1. A quantum system is initially prepared in $|\alpha_i\rangle$.
2. The system evolves under a unitary interaction $\hat{U}$ with a thermal bath $\hat{\rho}_{\mathrm{th}}$.
3. We then measure the overlap between the final state and $|\alpha_f\rangle$

Transition probability then leads to $P_{\rightarrow}(\alpha_f|\alpha_i) = \mathrm{Tr}\left[\hat{U}(|\alpha_i\rangle\langle\alpha_i| \otimes \hat{\rho}_{\mathrm{th}})\hat{U}^{\dagger}(|\alpha_f\rangle\langle\alpha_f| \otimes \mathbb{I})\right]$

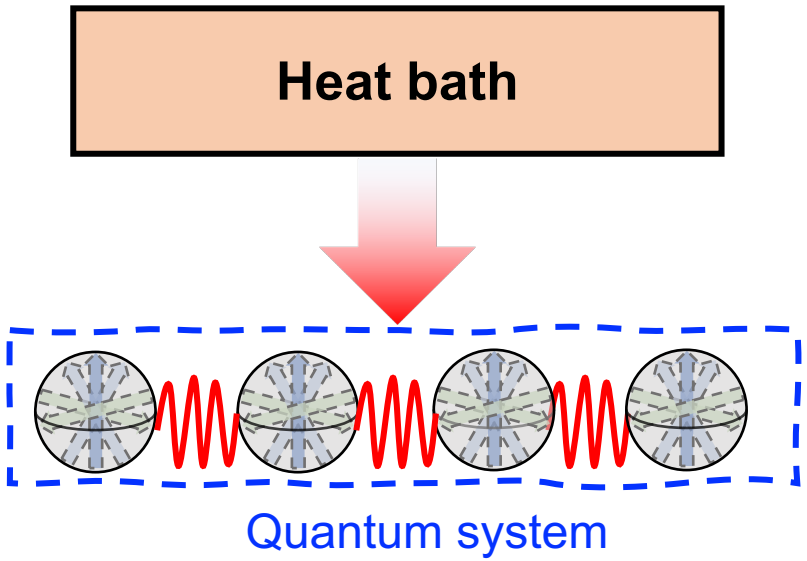
[Backward process]



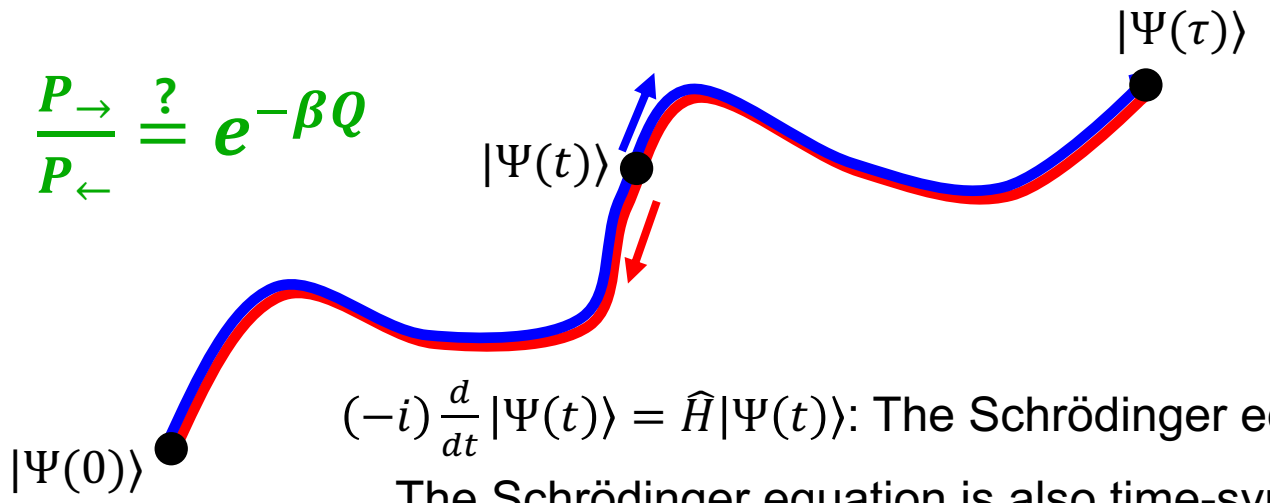
❖ Repeat 1-3 with the time-reversed initial/final states and unitary interaction $\hat{U}_R$.

Transition probability then leads to $P_{\leftarrow}(\alpha_i^*|\alpha_f^*) = \mathrm{Tr}\left[\hat{U}_R(|\alpha_f^*\rangle\langle\alpha_f^*| \otimes \hat{\rho}_{\mathrm{th}})\hat{U}_R^{\dagger}(|\alpha_i^*\rangle\langle\alpha_i^*| \otimes \mathbb{I})\right]$

Microscopic reversibility in quantum mechanics



$$\frac{P_{\rightarrow}}{P_{\leftarrow}} \stackrel{?}{=} e^{-\beta Q}$$



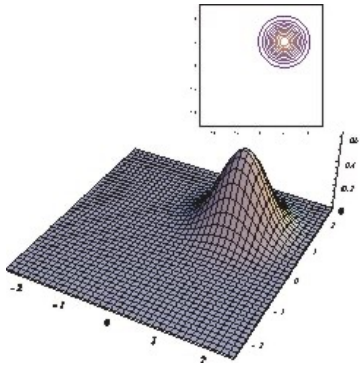
$(-i)\frac{d}{dt}|\Psi(t)\rangle = \hat{H}|\Psi(t)\rangle$: The Schrödinger equation

The Schrödinger equation is also time-symmetric

$t \rightarrow -t$ & $|\Psi\rangle \rightarrow |\Psi^*\rangle$

However, we cannot precisely determine $\hat{x}$ and $\hat{p}$ simultaneously as they do not commute to each other

$$[\hat{x}, \hat{p}] = i\hbar \Rightarrow \Delta x \Delta p \geq \hbar/2$$



The best description (with minimal uncertainty) we can make is using coherent states

(in a harmonic oscillator system: $\hat{H} = \frac{\hbar\omega_0}{2}(\hat{x}^2 + \hat{p}^2)$)

$$|\alpha\rangle = |\alpha_r + i\alpha_i\rangle = |x + ip\rangle$$

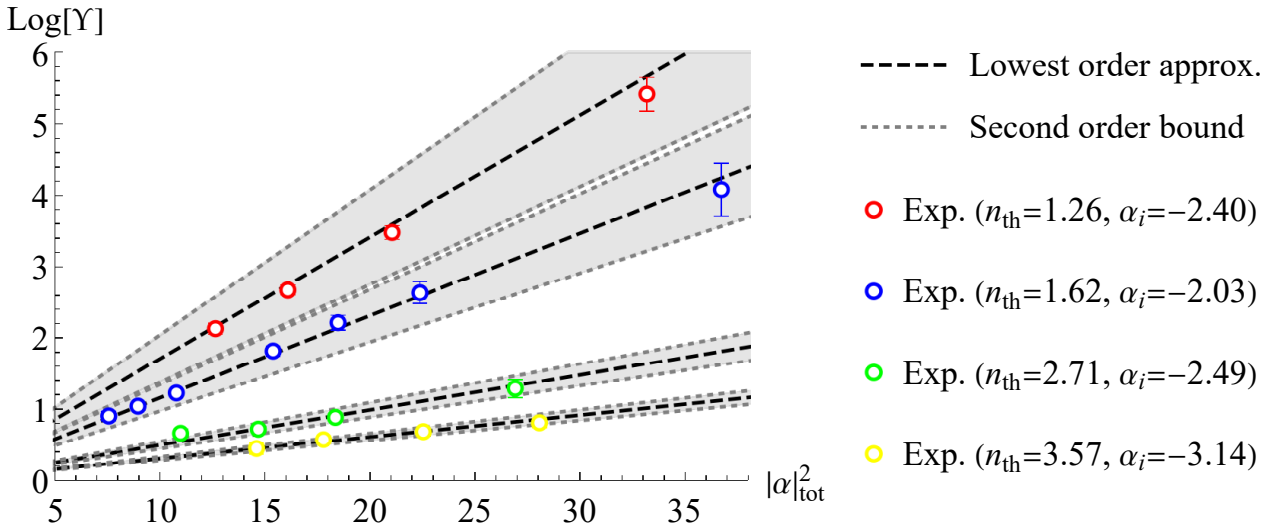
Will we have the same microscopic reversibility condition as in classical theory?

Experimental demonstration using quantum optics

$$\frac{P_{\rightarrow}(\alpha_f|\alpha_i)}{P_{\leftarrow}(\tilde{\alpha}_i|\tilde{\alpha}_f)} = \exp\left[-\frac{|\alpha_f|^2}{n_{\mathrm{th}}+1}+\frac{|\alpha_i|^2}{n_{\mathrm{th}}}\right] = \Upsilon e^{-\beta Q}$$

$$|\alpha|^2_{\mathrm{tot}} = |\alpha_i|^2 + |\alpha_f|^2$$

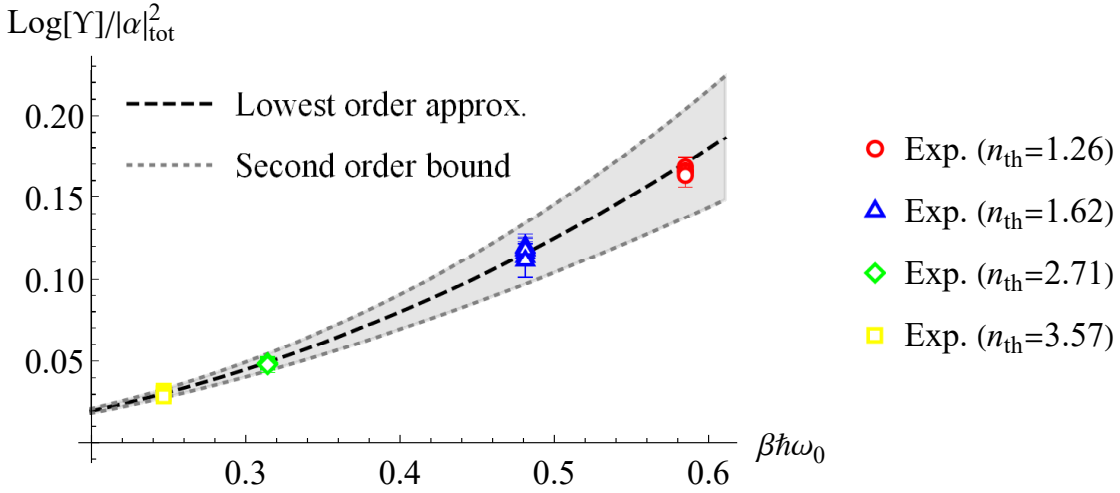
Deviation from the classical theory: $\log[\Upsilon] = [\cosh(\beta\hbar\omega_0)-1]|\alpha|^2_{\mathrm{tot}} - [\sinh(\beta\hbar\omega_0)-\beta\hbar\omega_0]\Delta|\alpha|^2 \approx \frac{(\beta\hbar\omega_0)^2}{2}|\alpha|^2_{\mathrm{tot}}$



Quantum correction increases when $|\alpha_i|\&|\alpha_f|$ increases

$$|\alpha\rangle = e^{-\frac{|\alpha|^2}{2}}\sum_{n=0}^{\infty}\frac{\alpha^n}{\sqrt{n!}}|n\rangle$$

The larger the $|\alpha|$, the larger the coherence



Quantum to classical transition when the temperature becomes high

$$\left(\beta = \frac{1}{k_B T} \approx 0 \text{ or } n_{\mathrm{th}} \gg 1\right)$$

For more detail: M. Bellini, HK, *et al.*, to appear in PRL

Outline

- **Quantum thermodynamics**
- **Microscopic description of the second law**
- **Quantum microscopic reversibility condition**
- **Conclusion**

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