Emergent Fluctuation Theorem for Pure Quantum States

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YKIS2016: Quantum Matter, Spacetime and Information

Kazuya Kaneko

Eiki Iyoda

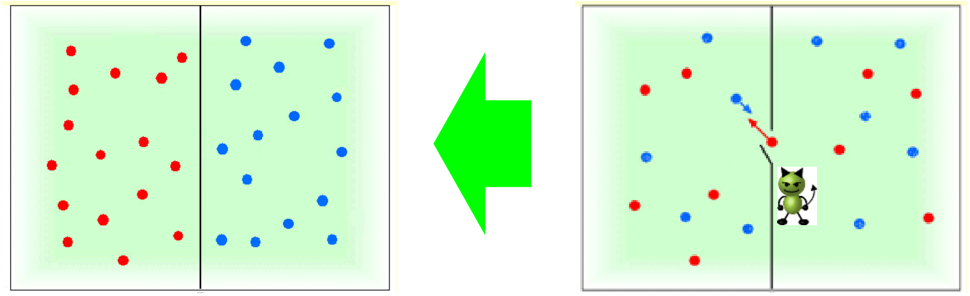
arXiv:1603.07857

Have been working on…

- Nonequilibrium statistical physics

- Quantum information theory

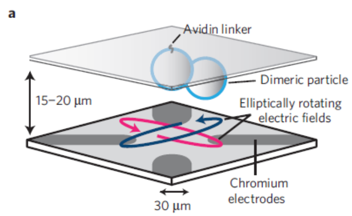
In particular, **thermodynamics of information**

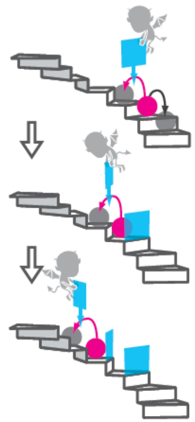


Maxwell's demon

Thermodynamics of Information

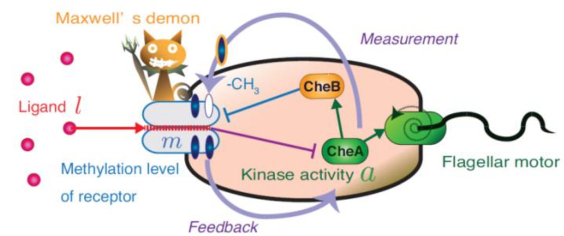
Information processing at the level of thermal fluctuations





Experimental realization of Maxwell's demon:
Toyabe, Sagawa, Ueda, Muneyuki, Sano, *Nature Physics* (2010)

E. Coli chemotaxis



Ito & Sagawa, *Nature Communications* (2015)

Review: **J. M. R. Parrondo, J. M. Horowitz, & T. Sagawa, *Nature Physics* 11, 131-139 (2015).**

A related fundamental issue:

How does thermodynamics (and its connection to information) emerge in purely quantum systems?

Today's topic!

Outline

- Introduction
- Review of fluctuation theorem

Our results:

- Second law
- Fluctuation theorem
- Numerical check

- Summary

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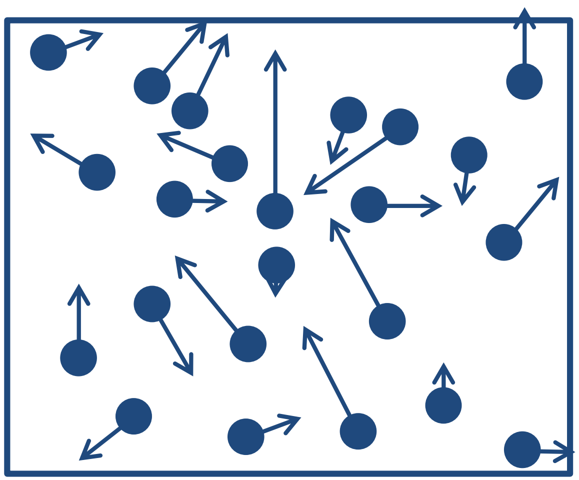
Origin of macroscopic irreversibility

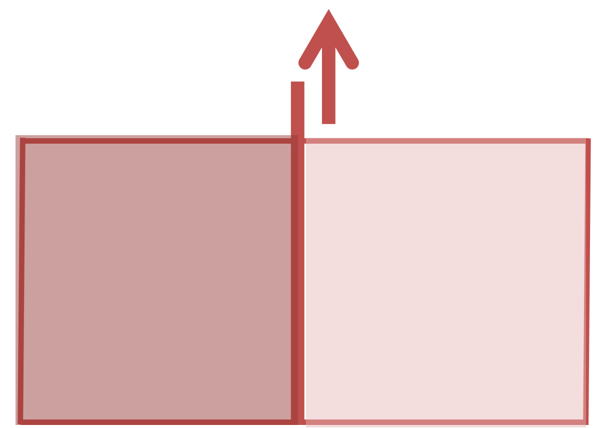
micro (Quantum mechanics)

reversible (unitary)



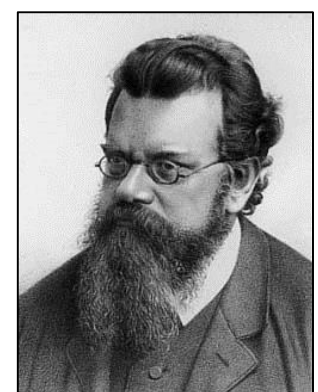
MACRO (Thermodynamics)

irreversible $\Delta S > 0$



"How does the macroscopic irreversibility emerge from microscopic dynamics?"

→ Fundamental question since Boltzmann



Relaxation in isolated quantum systems

Microscopically reversible unitary dynamics

→ **Relaxes towards a macroscopic steady state**

（Recurrence time is very long: almost irreversible!）

$|\Psi(0)\rangle$ **Non-steady** pure state

$\downarrow \hat{U} = \exp(-i\hat{H}t)$ ：Unitary

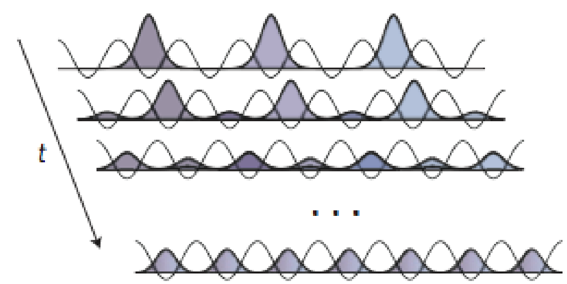
$|\Psi(t)\rangle$ **Macroscopically steady** pure state

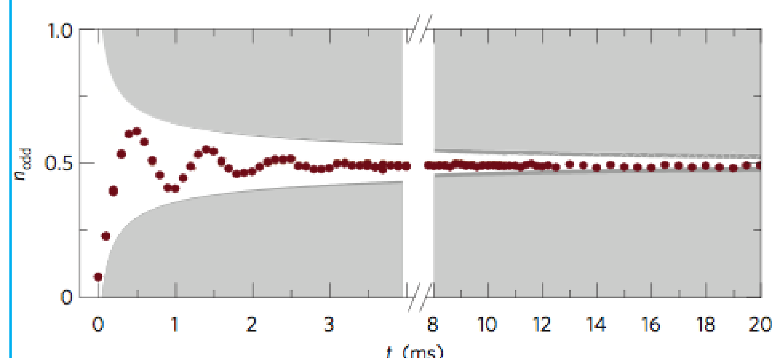
Rigorous proof for arbitrary initial states

Von Neumann, 1929 (arXiv:1003.2133)

Experiment：Ultracold atoms

ex. 1d Bose-Hubbard, ^{87}Rb





S. Trotzky et al., Nature physics **8**, 325 (2012)

Info. entropy vs thermo. entropy

Macroscopically irreversible relaxation emerges from microscopically reversible unitary dynamics

Information entropy

$$\mathrm{D}S = 0$$

$$S(t) = \mathrm{tr}\left[-\hat{r}(t)\ln\hat{r}(t)\right]$$

von Neumann entropy

: invariant under

unitary time evolution

$$\xleftrightarrow{\quad ? \quad}$$

Thermodynamic entropy

$$\mathrm{D}S_{\mathrm{thermo}} > 0$$

$$S_{\mathrm{thermo}} = k_{\mathrm{B}} \ln W$$

Increases under

irreversible processes

W : determined by Hamiltonian

Fundamental **GAP** between

information/thermodynamics entropy

Our results

Iyoda, Kaneko, Sagawa,
arXiv:1603.07857

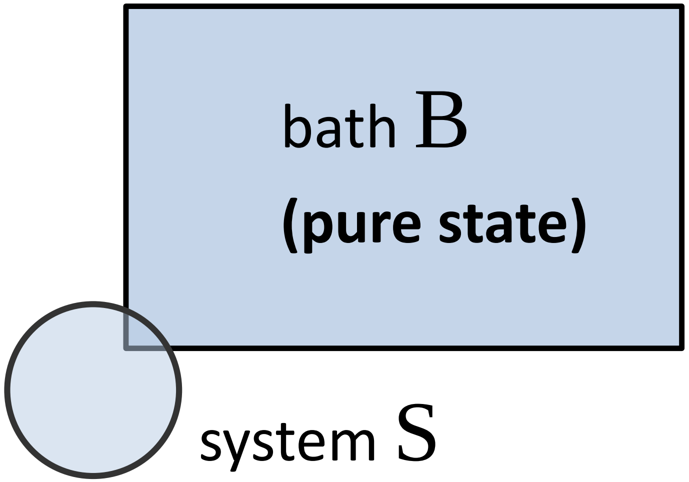
For pure states under reversible unitary dynamics, within small errors

✓ **2nd Law** $$\Delta S_{\mathrm{S}} \geq \beta \langle Q \rangle$$

relates von Neumann entropy

to thermodynamic heat

→ **Information-thermodynamics link**



✓ **The fluctuation theorem** $$\frac{P_{\mathrm{F}}(\sigma)}{P_{\mathrm{R}}(-\sigma)} = e^{\sigma}$$

σ : entropy production

characterizes fundamental symmetry of entropy production

→ **Thermal fluctuation emerges from quantum fluctuation**

Mathematically rigorous proof + Numerical check

Key idea: **Lieb-Robinson bound**, based on locality of interactions

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Second law and fluctuation theorem

2nd law

Entropy production is non-negative on average

$$\langle s \rangle \geq 0$$

Fluctuation theorem

Universal relation far from equilibrium

$$\frac{P_{\mathrm{F}}(s)}{P_{\mathrm{R}}(-s)} = e^{s}$$

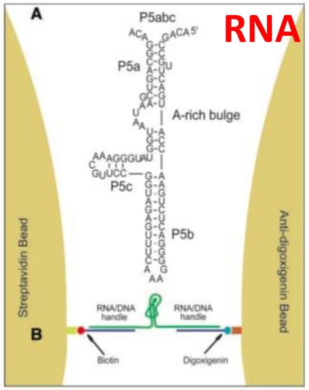
Probabilities of Positive/negative entropy productions

Second law as an **equality**!

Theory（1990's-）
Dissipative dynamical systems,
Classical Hamiltonian systems,
Classical Markov (ex. Langevin),
Quantum Unitary, Quantum Markov, …

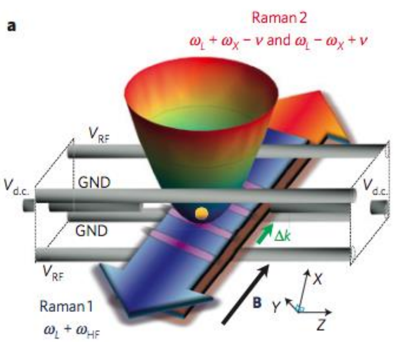
Experiment（2000's-）
Colloidal particle, Biopolymer,
Single electron, Ion trap, NMR, …

Classical



J. Liphardt et al.,
Science **296**, 1832 (2002)

Quantum (Ion-trap)



A. An et al.,
Nat. phys. **11**, 193 (2015)

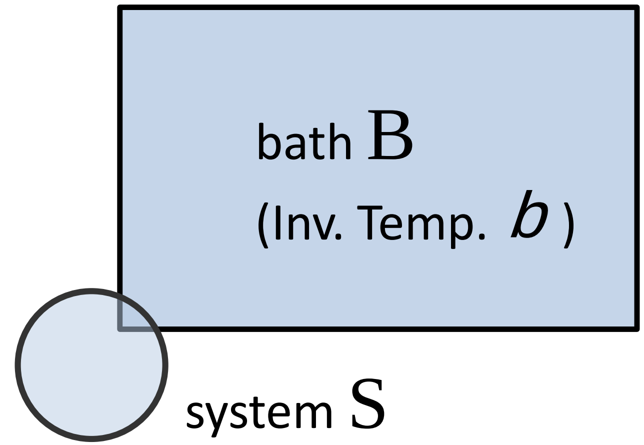
Setup for previous studies

By J. Kurchan, H. Tasaki, C. Jarzynski, …

Total system: system S and bath B

S+B obeys unitary dynamics

$$\hat{r}(t) = \hat{U}\hat{r}(0)\hat{U}^{\dagger}, \quad \hat{U} = \exp(-\,i\hat{H}t)$$



- Initial state of S: arbitrary
- **Initial state of B: Canonical**
  - **→ This assumption effectively breaks time reversal symmetry.**
- No initial correlation between S and B.

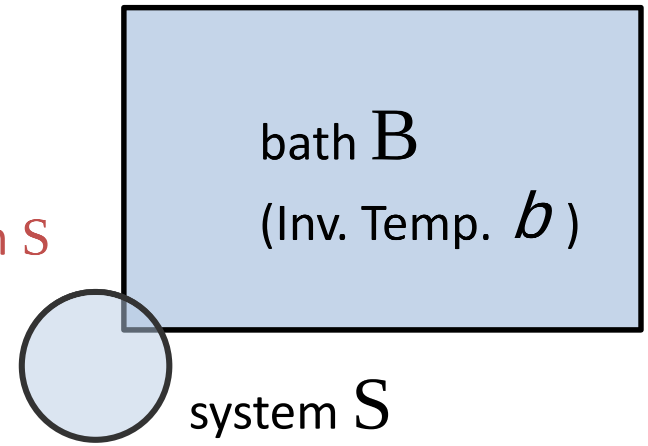
$$\hat{r}(0) = \hat{r}_{\mathrm{S}}(0)\,\ddot{\mathrm{A}}\,\hat{r}_{\mathrm{B}}(0), \quad \hat{r}_{\mathrm{B}}(0) = e^{-\,b\hat{H}_B} / Z_B$$

Second law (Clausius inequality)

$$\Delta S_{\mathrm{S}} \geq \beta \langle Q \rangle$$

heat absorbed by system S

Change in the von Neumann entropy of system S (Information entropy)



$$S_{\mathrm{S}}(t) = \mathrm{tr}_{\mathrm{S}}\left[-\hat{\rho}_{\mathrm{S}}(t)\ln\hat{\rho}_{\mathrm{S}}(t)\right], \quad \hat{\rho}_{\mathrm{S}}(t) = \mathrm{tr}_{\mathrm{B}}\left[\hat{\rho}(t)\right]$$

$\langle Q \rangle = -\,\mathrm{tr}_{\mathrm{B}}\left[(\hat{\rho}(t) - \hat{\rho}(0))\hat{H}_{\mathrm{B}}\right]$: heat absorbed by system S

Information entropy and **Heat** are linked!

（if the initial state of bath B is **canonical**）

Fluctuation theorem

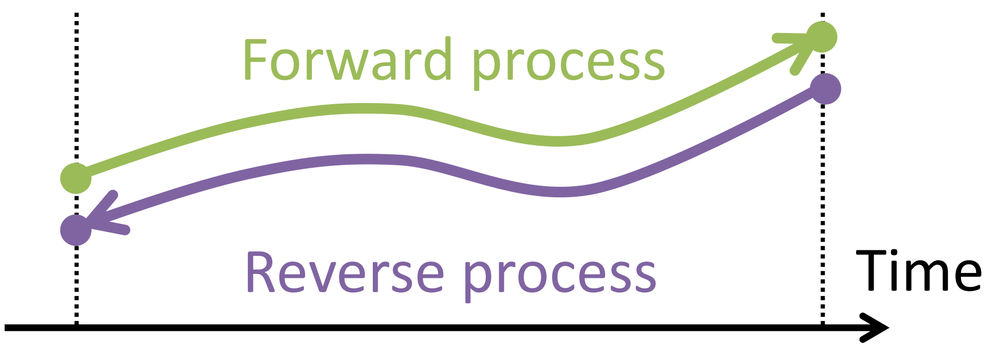
$\langle \sigma \rangle \equiv \Delta S_{\mathrm{S}} - \beta \langle Q \rangle \geq 0$: entropy production on average (non-negative)

σ : stochastic entropy production (fluctuates)

Let $\hat{\sigma}(t) \equiv -\ln \rho_{\mathrm{S}}(t) + \beta \hat{H}_B$
Projection measurements of $\hat{\sigma}(t)$ at initial and final time
Difference of outcomes: σ

Fluctuation theorem universally characterizes the ratio between the probabilities of positive/negative entropy productions

$$\frac{P_{\mathrm{F}}(s)}{P_{\mathrm{R}}(-s)} = e^{s}$$



Fluctuation theorem

Another representation with characteristic function (moment generating function)

$$\boxed{G_{\mathrm{F}}(u) = G_{\mathrm{R}}(-u+i)} \quad \xleftrightarrow{\text{Fourier transf.}} \quad \frac{P_{\mathrm{F}}(s)}{P_{\mathrm{R}}(-s)} = e^{s}$$

$$G_{\mathrm{F/R}}(u) = \int_{-\infty}^{+\infty} d\sigma e^{iu\sigma} P_{\mathrm{F/R}}(\sigma)$$: Fourier transf. of probability distribution

Cf. Fluctuation theorem leads to several important relations

Fluctuation theorem **Jarzynski identity** **Second law**

$$P_{\mathrm{F}}(s) = P_{\mathrm{R}}(-s)e^{s} \xrightarrow{\text{Integrate}} \langle \exp(-s) \rangle = 1 \xrightarrow{\text{Jensen inequality (convexity)}} \langle s \rangle \geq 0$$

Also reproduces the Green-Kubo formula in the linear response regime, and its higher order generalization

Second law with pure state bath?

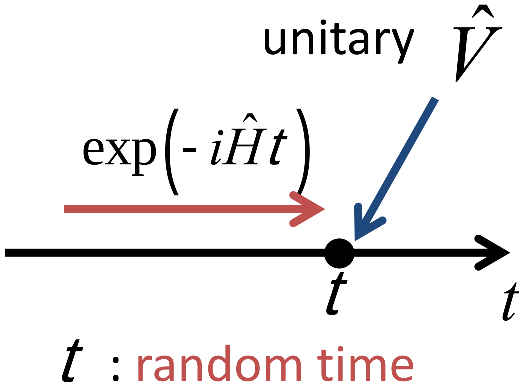
In the conventional argument, the initial **canonical** distribution of the bath is assumed, which effectively breaks the time-reversal symmetry.

➡ The origin of irreversibility was not fully understood, and thus we should consider **pure state baths**.

A few previous works (on the second law):

→ **Assumption of "random waiting time"**

: similar effect to dephasing



H. Tasaki, arXiv:0011321 (2000)

S. Goldstein, T. Hara, and H. Tasaki, arXiv:1303.6393 (2013)

T. N. Ikeda, N. Sakumichi, A. Polkovnikov, and M. Ueda, Ann. Phys. **354**, 338 (2015)

Information-thermodynamics link and the fluctuation theorem for pure state baths were open problems.

Outline

- Introduction
- Review of fluctuation theorem

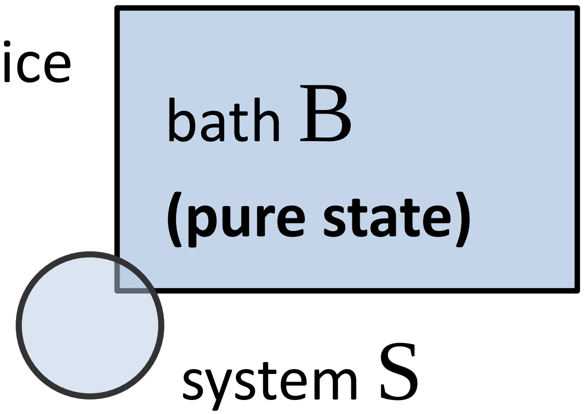
Our results:

- Second law
- Fluctuation theorem
- Numerical check

- Summary

Setup: system and bath

- Bath B: quantum many body system on a lattice
- Interaction: **local** and translational invariant
- Correlation in B is exponential decaying
- System S contacts with a part of bath B



- **Initial state of B: a typical pure state**

$$\hat{\rho}_{\mathrm{B}} = |\Psi\rangle\langle\Psi|$$

- No initial correlation between system and bath $\hat{\rho}(0) = \hat{\rho}_{\mathrm{S}}(0) \otimes \hat{\rho}_{\mathrm{B}}$

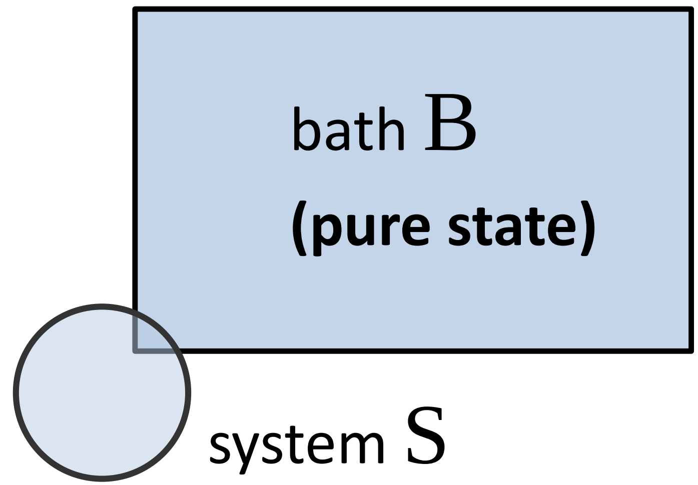
- Temperature of bath B

  is define by the temperature of the canonical distribution whose energy density is equal to the pure state

Setup: time evolution

- **Unitary time evolution:**

$$\hat{r}(t) = \hat{U}\hat{r}(0)\hat{U}^{\dagger}, \quad \hat{U} = \exp\left(- i\hat{H}t\right)$$



- **Relaxation after quench:**

Hamiltonian of S changes quickly at $t = 0$

and is time-independent for $t > 0$

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Second law (Clausius inequality)

$$\boxed{\Delta S_{\mathrm{S}} - \beta\langle Q\rangle \geq -\varepsilon_{\mathrm{2nd}}}$$

$S_{\mathrm{S}}(t) = \mathrm{tr}_{\mathrm{S}}\left[-\hat{\rho}_{\mathrm{S}}(t)\ln\hat{\rho}_{\mathrm{S}}(t)\right]$: von Neumann entropy of system S

$\langle Q\rangle = -\mathrm{tr}_{\mathrm{B}}\left[(\hat{\rho}(t) - \hat{\rho}(0))\hat{H}_{\mathrm{B}}\right]$: heat absorbed by system S

e_{2nd} **: Error term, vanishing in the large bath limit**

For any $\varepsilon_{\mathrm{2nd}} > 0$, for any t, there exists a sufficiently large bath, such that 2nd law holds.

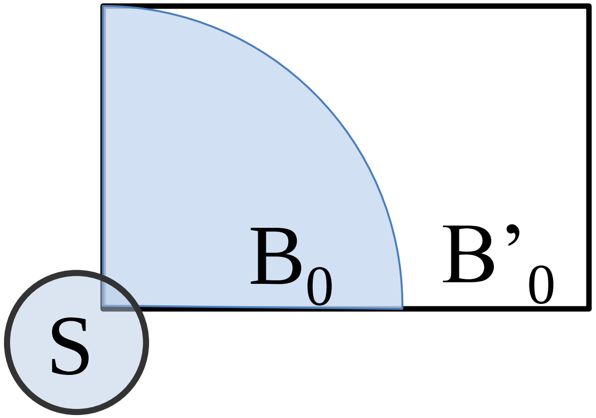
→ **Mathematically rigorous**

Even though the state of B is pure,

information and thermodynamics are linked!

Key of the proof: typicality

Reduced density operator of
a **typical pure state** $|\Psi\rangle$
(with respect to the **uniform measure** in the Hilbert space of the microcanonical energy shell)

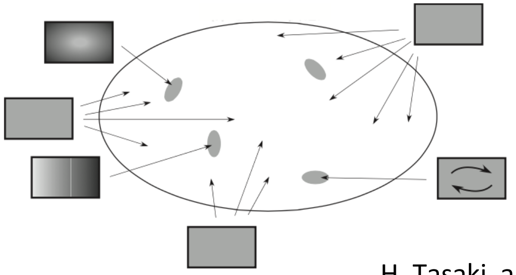


$$\rho_{B_0} \equiv \mathrm{tr}_{B'_0}\left[|\Psi\rangle\langle\Psi|\right]$$

is nearly equal to **canonical distribution**
(When B'_0 is large, the error is small)

S. Popescu *et al*., Nature physics (2006)
A. Sugita, RIMS Kokyuroku (2006)
S. Lloyd, Ph.D. Thesis

Almost all pure states are locally thermal!



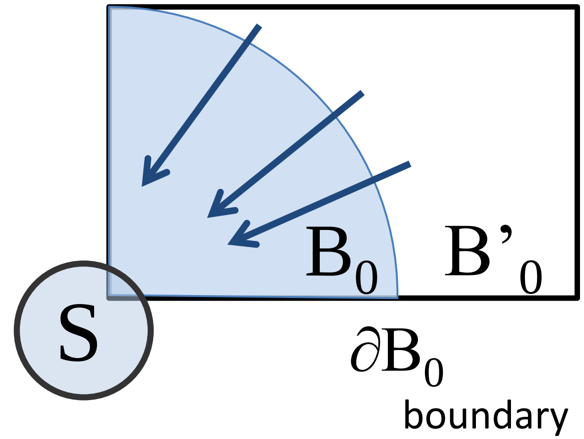
H. Tasaki, arXiv:1507.06479,(2015)

→ Origin of thermodynamic entropy of B_0 is the **entanglement entropy**

Key of the proof: Lieb-Robinson bound

The velocity of "information propagation" in B is finite, due to locality of interaction

Effective **"light-cone"** like structure



➡ S is not affected by $\mathrm{B'}_0$ in the short time regime

Lieb-Robinson bound

$$\left\| \left[\hat{O}_{\mathrm{S}}(t), \hat{O}_{\partial\mathrm{B}_0}\right] \right\| \le C \left\|\hat{O}_{\mathrm{S}}\right\| \cdot \left\|\hat{O}_{\partial\mathrm{B}_0}\right\| \cdot |S| \cdot |\partial\mathrm{B}_0| \cdot \exp\left[-\mu\,\mathrm{dist}(\mathrm{S},\partial\mathrm{B}_0)\right]\left(\exp(v|t|)-1\right)$$

$t \ll \tau \equiv \eta\,\mathrm{dist}(\mathrm{S},\partial\mathrm{B}_0)/v$ → small

v/η : Lieb-Robinson velocity

τ Lieb-Robinson time

E. Lieb and D. Robinson, Commun. Math. Phys. 28, 251 (1972)

M. Hastings and T. Koma, Commun. Math. Phys. 265, 781 (2006)

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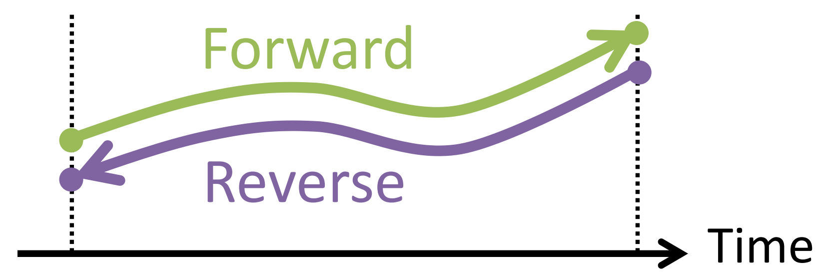
Fluctuation theorem: setup

$$\langle \sigma \rangle \equiv \Delta S_{\mathrm{S}} - \beta \langle Q \rangle \geq 0$$: entropy production on average (non-negative)

σ : stochastic entropy production (fluctuates)

Let $\hat{\sigma}(t) \equiv -\ln \rho_{\mathrm{S}}(t) + \beta \hat{H}_B$
Projection measurements of $\hat{\sigma}(t)$ at initial and final time
Difference of outcomes: σ

Moment generating function for entropy production
(F: Forward, R: Reverse)



$$G_{\mathrm{F/R}}(u) = \int_{-\infty}^{+\infty} d\sigma\, e^{iu\sigma} P_{\mathrm{F/R}}(\sigma)$$

Initial state of the reverse process: $\hat{\rho}_{\mathrm{S}}(t) \otimes \hat{\rho}_{\mathrm{B}}$

Same as the initial state of forward process

Result: Fluctuation theorem

$$\left| G_{\mathrm{F}}(u) - G_{\mathrm{R}}(-u+i) \right| \leq \varepsilon_{\mathrm{FT}} \quad \xleftrightarrow{\text{Fourier Transf.}} \quad \frac{P_{\mathrm{F}}(\sigma)}{P_{\mathrm{R}}(-\sigma)} \cong e^{\sigma}$$

For any $\varepsilon_{\mathrm{FT}} > 0$, for any time t, there exists a sufficiently large bath, such that…

→ **Mathematically rigorous**

In addition, $[H_{\mathrm{S}} + H_{\mathrm{B}}, H_{\mathrm{I}}] = 0$ is assumed.
If this commutator is not zero but small,
a small correction term is needed.

Universal property of thermal fluctuation far from equilibrium emerges from quantum fluctuation of pure states!

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Numerical check

Second law $\langle \sigma \rangle \geq -\varepsilon_{\mathrm{2nd}}$

Fluctuation theorem $\left| G_{\mathrm{F}}(u) - G_{\mathrm{R}}(-u+i) \right| \leq \varepsilon_{\mathrm{FT}}$

Error estimation is mathematically rigorous
（For any error and time, 2nd law and FT hold for sufficiently large bath.）
→ However, it is not trivial whether the errors are small in realistic situations.

→ We confirm that the second law and FT hold
even with a very small bath (16 sites)

System and Hamiltonian

Hard core bosons with n.n. repulsion on 2-dim square lattice

$$\hat{H} = \underbrace{\sum_{i} \epsilon_i \hat{c}_i^{\dagger} \hat{c}_i}_{\text{Potential}} + \underbrace{\sum_{\langle i,j \rangle} (-\gamma_{ij}) \left(\hat{c}_i^{\dagger} \hat{c}_j + \hat{c}_j^{\dagger} \hat{c}_i \right)}_{\text{Hopping}} + \underbrace{\sum_{\langle i,j \rangle} g_{ij} \hat{c}_i^{\dagger} \hat{c}_i \hat{c}_j^{\dagger} \hat{c}_j}_{\text{Repulsion}}$$

$$g_{ij} = g,\ \gamma_{ij} = \gamma \quad (i, j \in B)$$

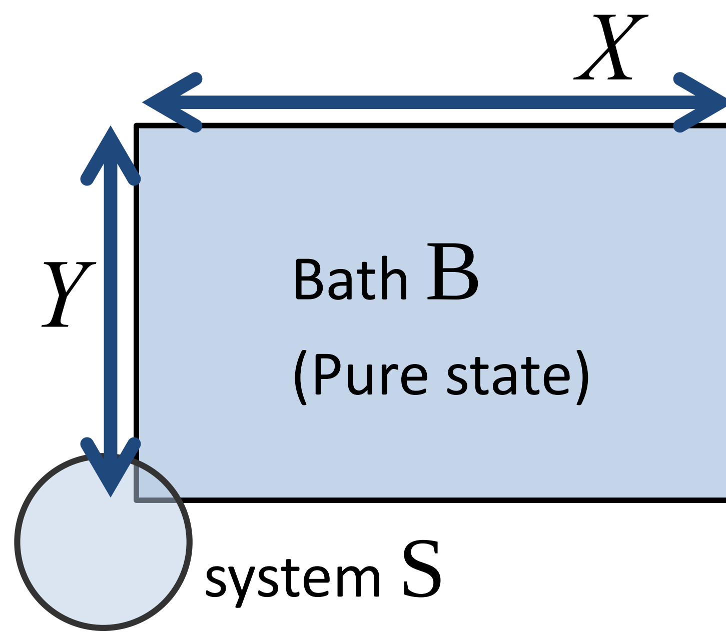
$$g_{ij} = 0,\ \gamma_{ij} = \gamma' \quad (\text{otherwise})$$

$\epsilon_i = \epsilon$ ← unit of energy

Bath: $X \times Y$ sites, #particles=N

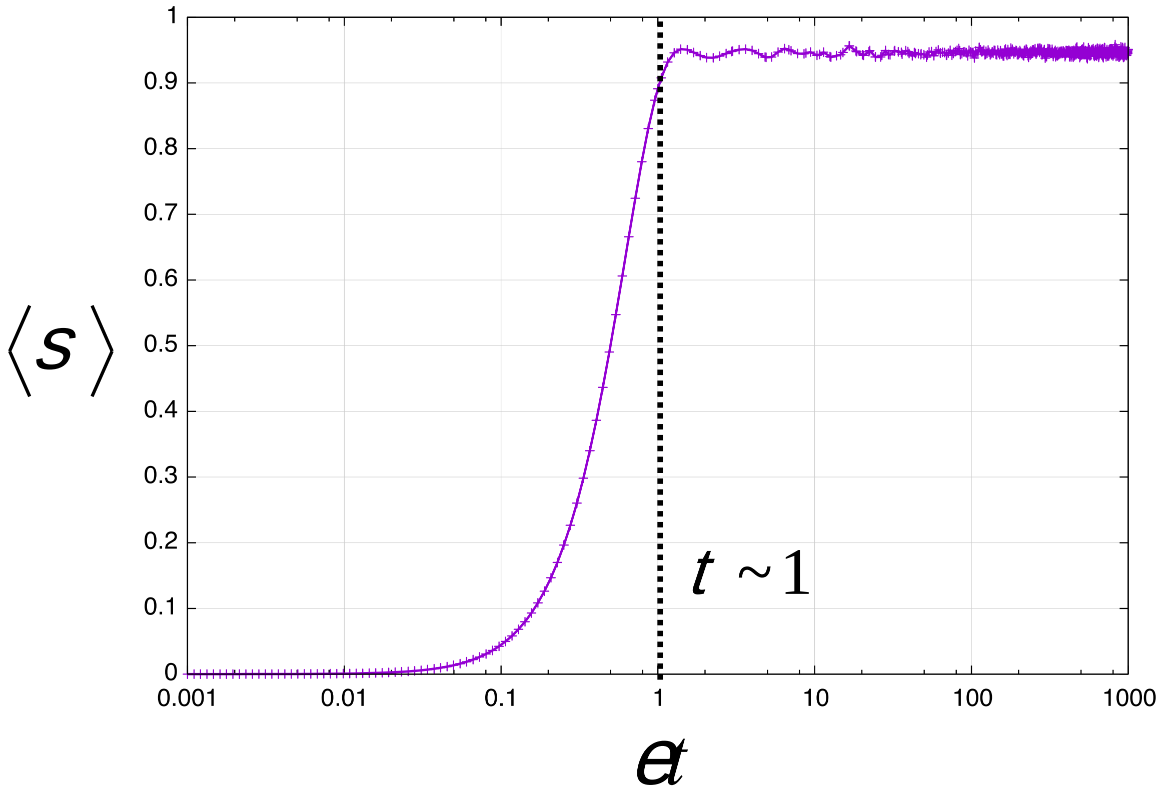
System: 1 site

Initial state: $\hat{\rho}_{\mathrm{S}}(0) = |1\rangle\langle 1|$



Method: Exact diagonalization (full)

Second law (1)



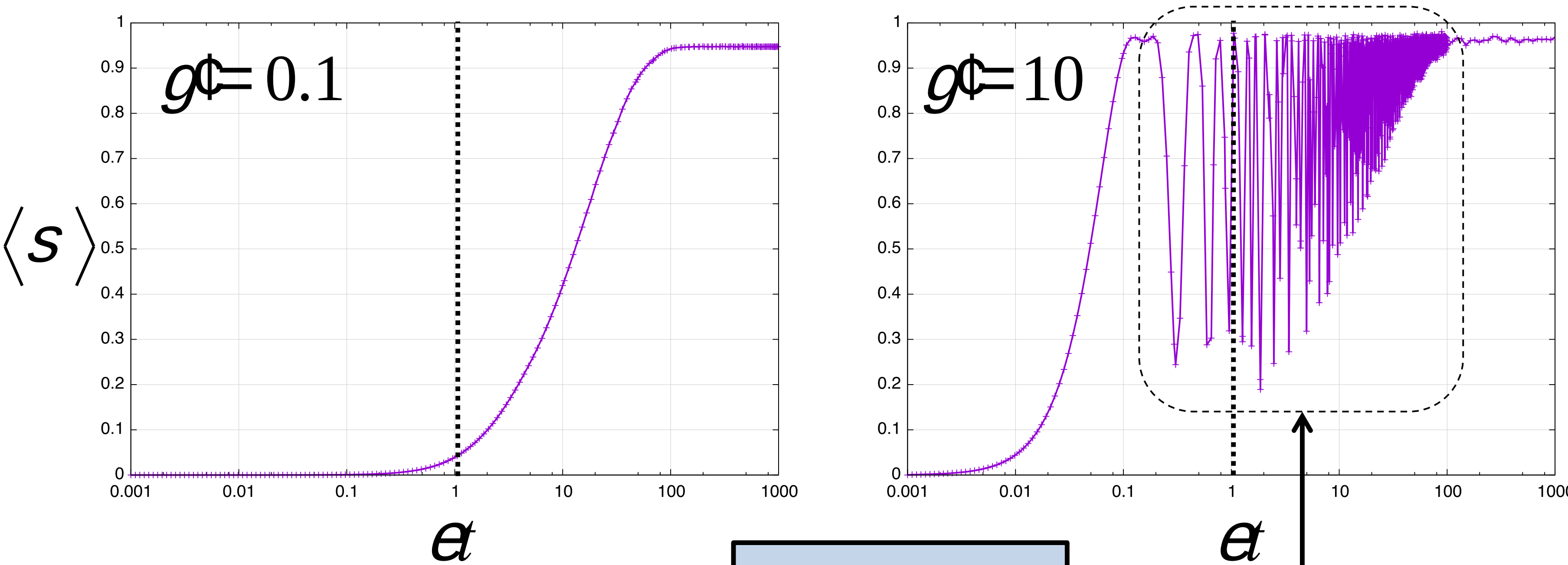
Lieb-Robinson time $\tau \sim 1$

parameters: $\epsilon=1,\ \gamma=1,\ \gamma'=1,\ g=0.1,\ (X,Y,N)=(4,4,5)$

Average entropy production is always non-negative

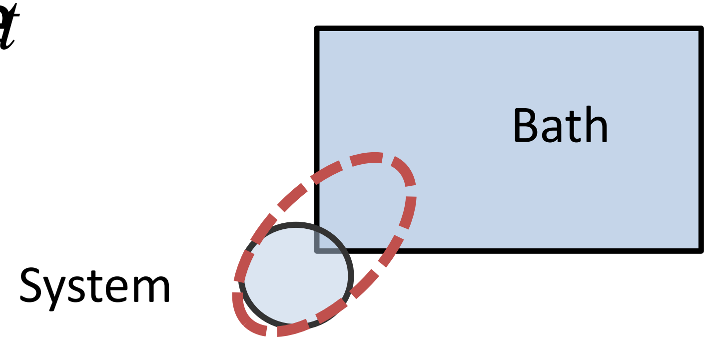
→ Second law holds (even beyond the Lieb-Robinson time!)

Second law (2)



Lieb-Robinson time

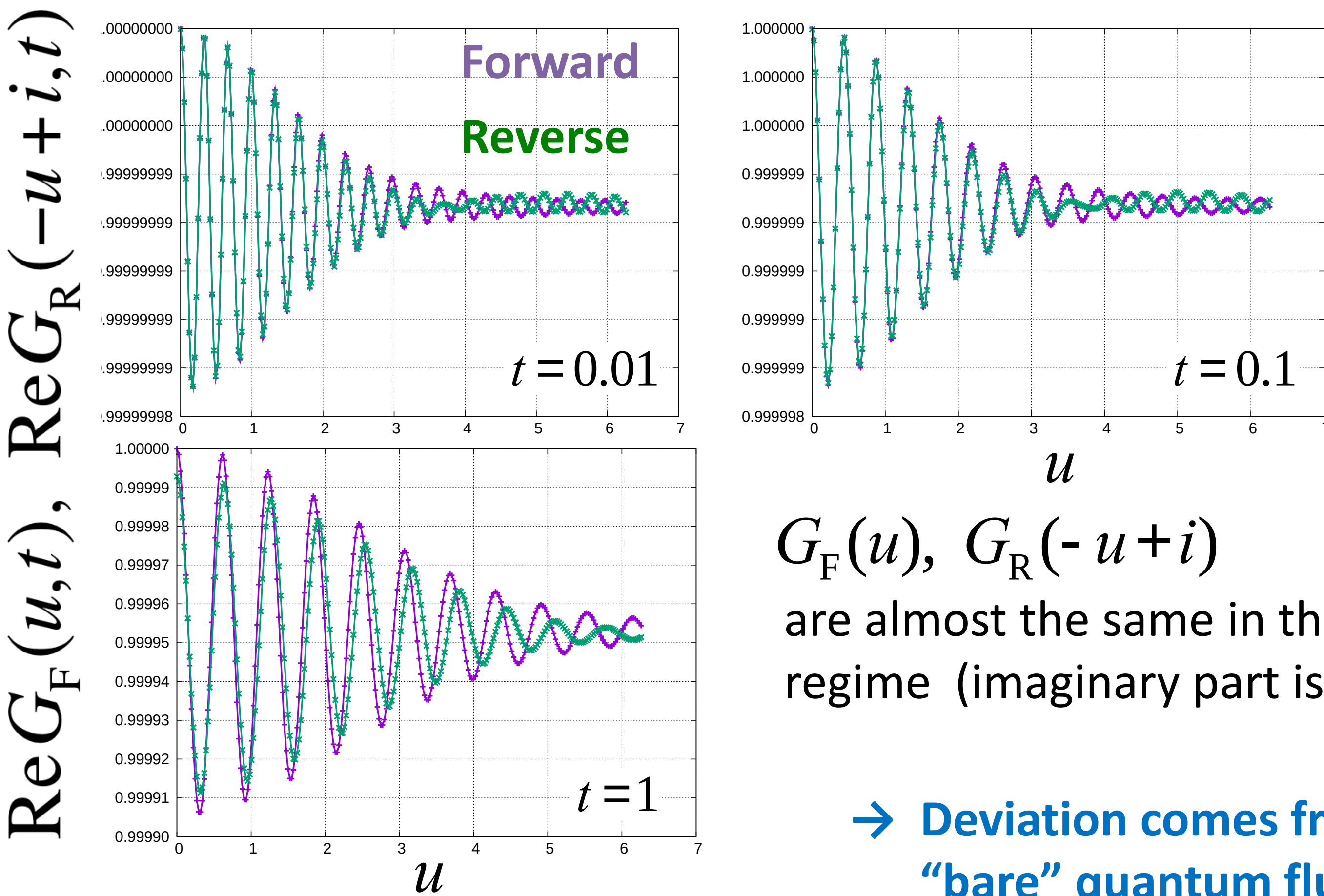
$\tau \sim 1$



Rabi oscillation between system S and Bath

parameters: $\epsilon = 1,\ g' = 1,\ g = 0.1,\ (X, Y, N) = (4, 4, 5)$

Fluctuation theorem (1)



Lieb-Robinson Time $t \sim \frac{1}{2}$

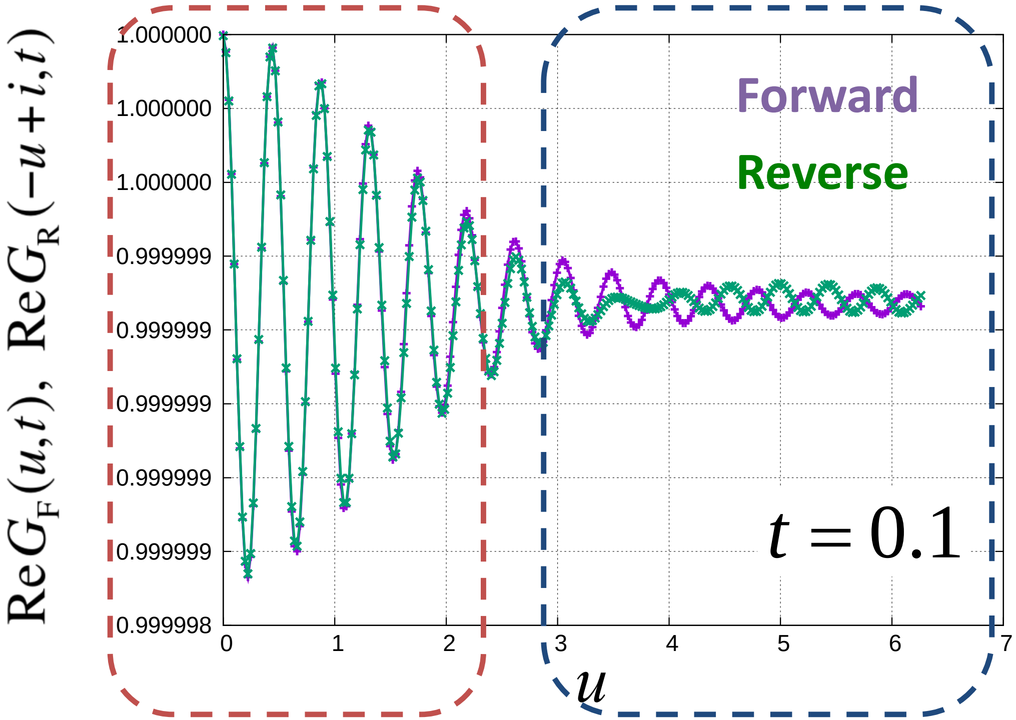
$G_{\mathrm{F}}(u),\ G_{\mathrm{R}}(-u+i)$ are almost the same in the short time regime (imaginary part is also the same)

→ **Deviation comes from "bare" quantum fluctuation**

(**Dynamical crossover** between thermal fluctuation and bare quantum fluctuation)

parameters: $e=1,\ g=2,\ g'=0.01,\ g=0.1,\ (X,Y,N)=(3,5,4)$

Fluctuation theorem (2)



Lower order moments

Higher order moments

nth moment

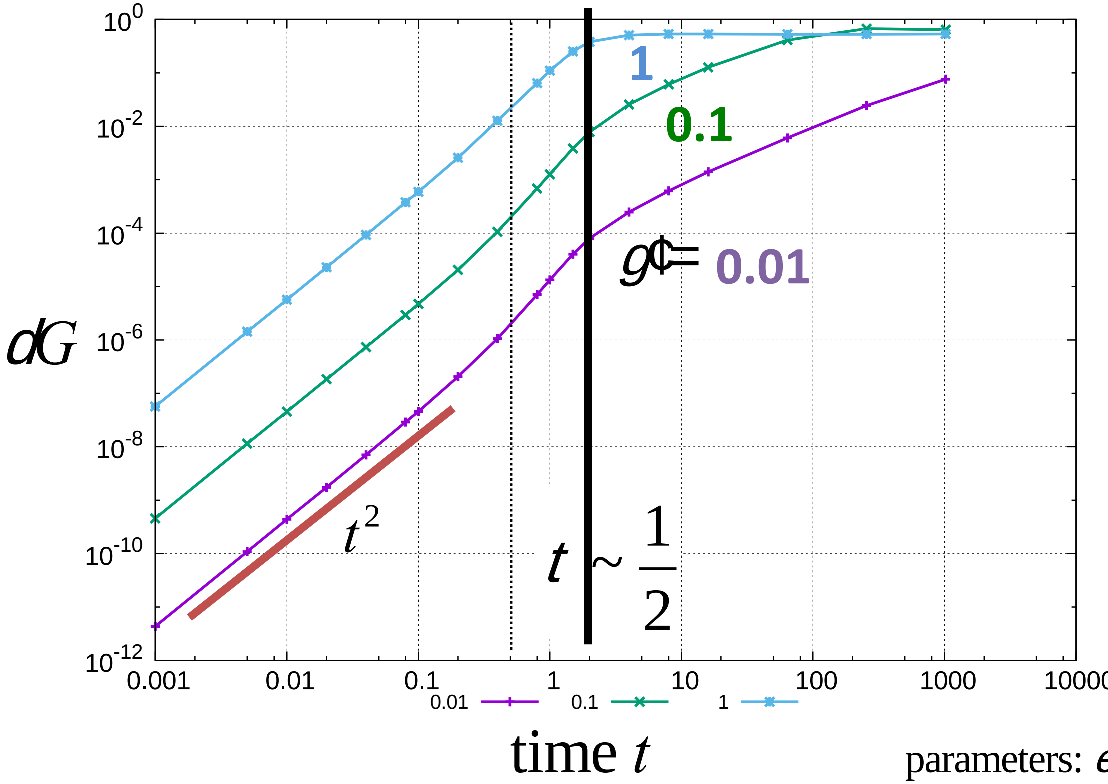
$$\left\langle \sigma^{n} \right\rangle_{\mathrm{c}} = \left.\frac{\partial^{n} G(u,t)}{\partial (iu)^{n}}\right|_{u=0}$$

→ Higher order moments deviate faster.

parameters: $e=1,\ g=2,\ g'=0.01,\ g=0.1,\ (X,Y,N)=(3,5,4)$

Fluctuation theorem: error estimation

Integrated error: $dG \equiv \int_0^{2p} du \left|G_F(u) - G_R(-u+i)\right|$



Lieb-Robinson Time

$t \sim \frac{1}{2}$

parameters: $e=1$, $g=2$, $g=0.1$, $(X,Y,N)=(3,5,4)$

Agrees with t^2 dependence predicted by our theory

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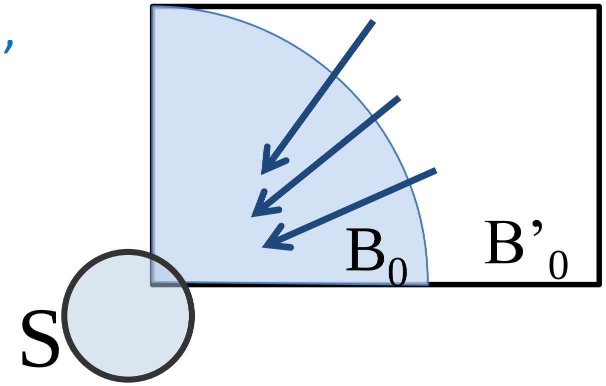
Summary

Iyoda, Kaneko, Sagawa, arXiv:1603.07857

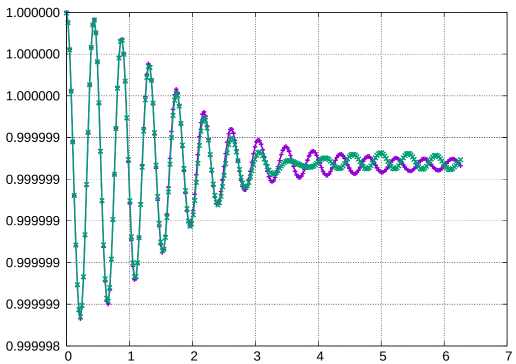


For pure states under reversible unitary dynamics,

✓ **Second law** $$\Delta S_{\mathrm{S}} - \beta\langle Q\rangle \geq -\varepsilon_{\mathrm{2nd}}$$

relates thermodynamic heat and the von Neumann entropy

→ **Information-thermodynamics link**



✓ **Fluctuation theorem** $$\left|G_{\mathrm{F}}(u) - G_{\mathrm{R}}(-u+i)\right| \le \epsilon_{\mathrm{FT}}$$

Fundamental symmetry of entropy production far from equilibrium

→ **Emergence of thermal fluctuation from quantum fluctuation**

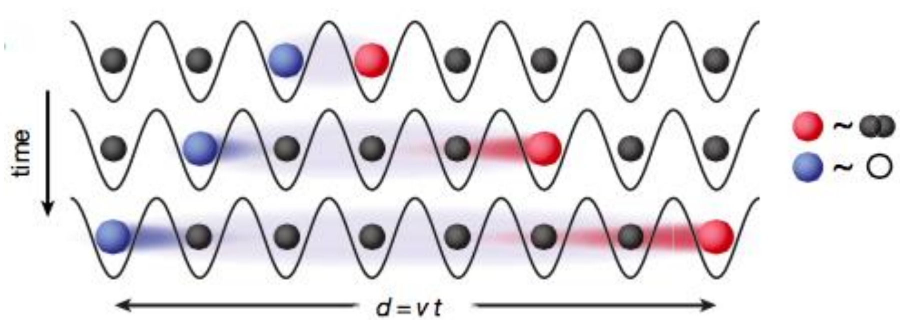
Mathematically rigorous proof ＋ Numerical check (Exact disgonalization)

Key idea: **Lieb-Robinson bound**

Perspectives

Possible experiments

→ **Ultracold atoms?**

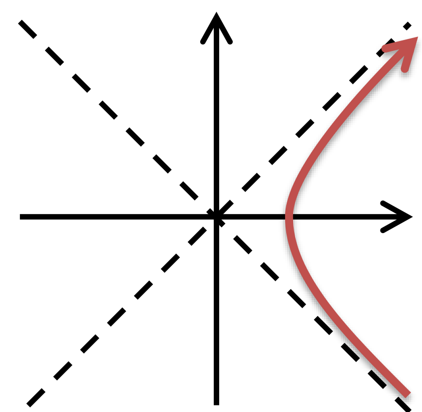


M. Cheneau *et al.*, Nature (2012)

Possible connection to quantum gravity

→ **Unruh & Hawking radiation?**

→ **"Fast scrambling" conjecture?**



Thank you for your attention!