# 孤立量子多体系の熱平衡化と第二法則

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2019年1月16日
量子多体系の素核・物性クロスオーバー @KEK

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E. Iyoda, K. Kaneko, T. Sagawa, PRL **119**, 100601 (2017).

T. Yoshizawa, E. Iyoda, T. Sagawa, PRL **120**, 200604 (2018).

# Outline

- Introduction
- Eigenstate thermalization hypothesis (ETH)
    - Review of ETH
    - Our result: Numerical large deviation analysis
- Second law and fluctuation theorem
    - Conventional setup
    - Our result: SL and FT for pure quantum states

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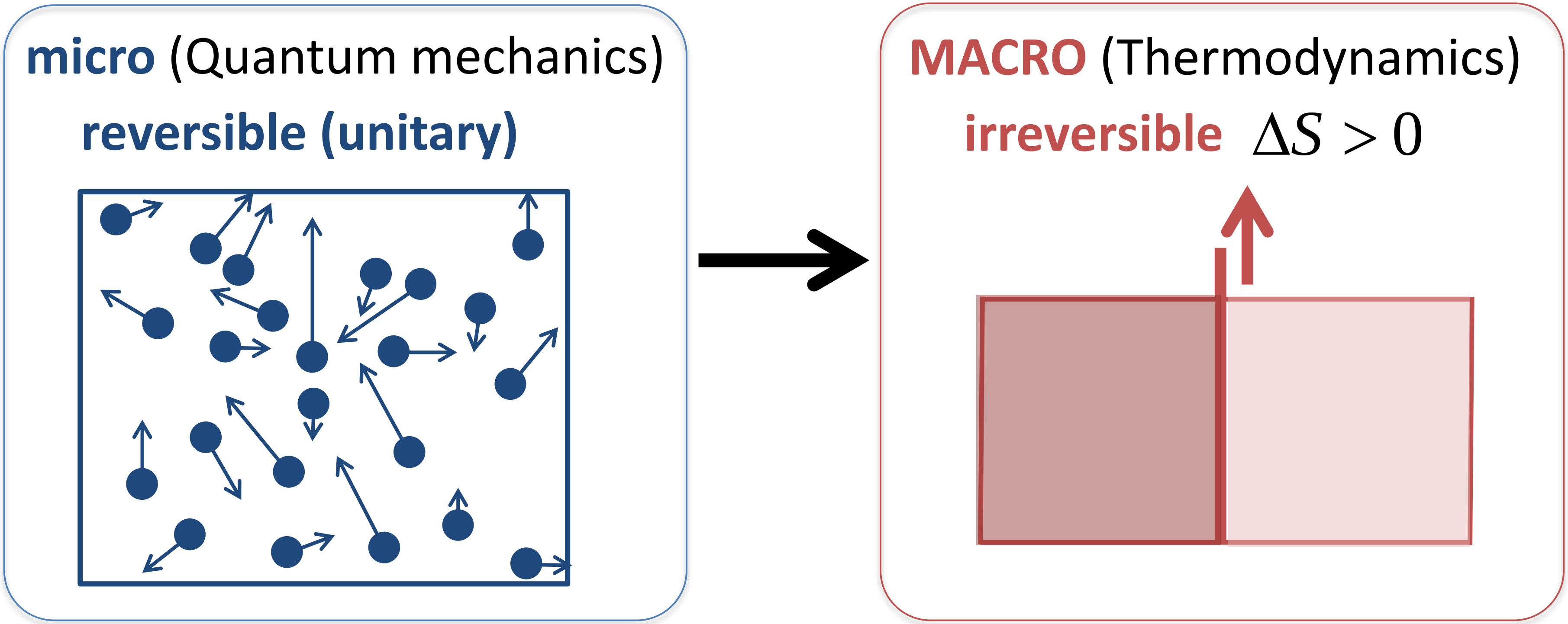
# Origin of macroscopic irreversibility



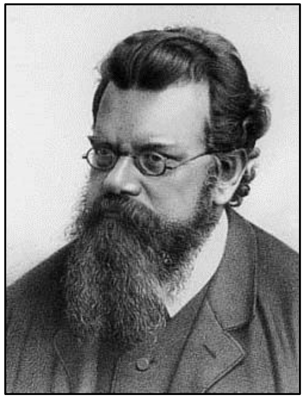
**micro** (Quantum mechanics)

**reversible (unitary)**

**MACRO** (Thermodynamics)

**irreversible** $\Delta S > 0$

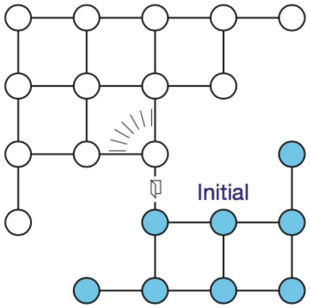
Fundamental question since Boltzmann



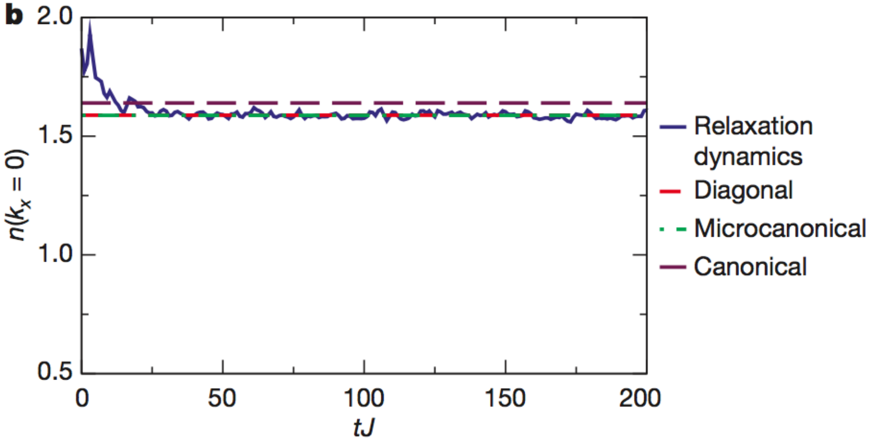
# Modern progress

**Numerical simulation:**

Exact diagonalization



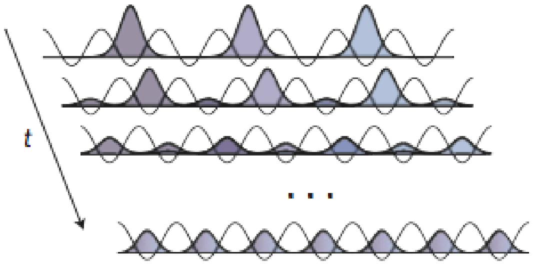
Hard-core bosons



M. Rigol et al., Nature **452**, 854 (2008)

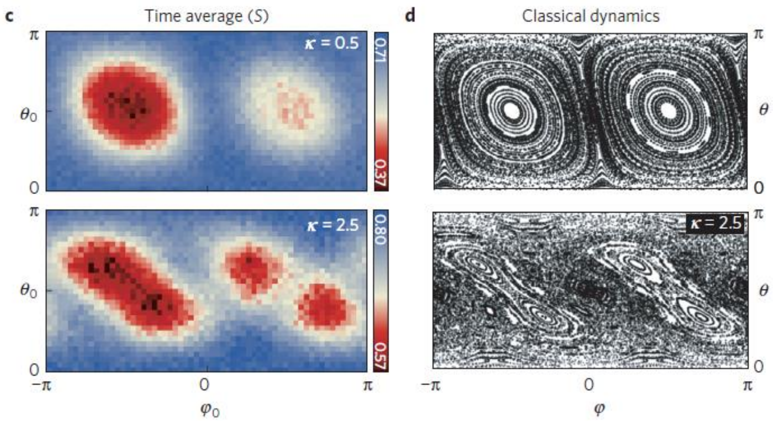
**Experiments:**

Ultracold atoms



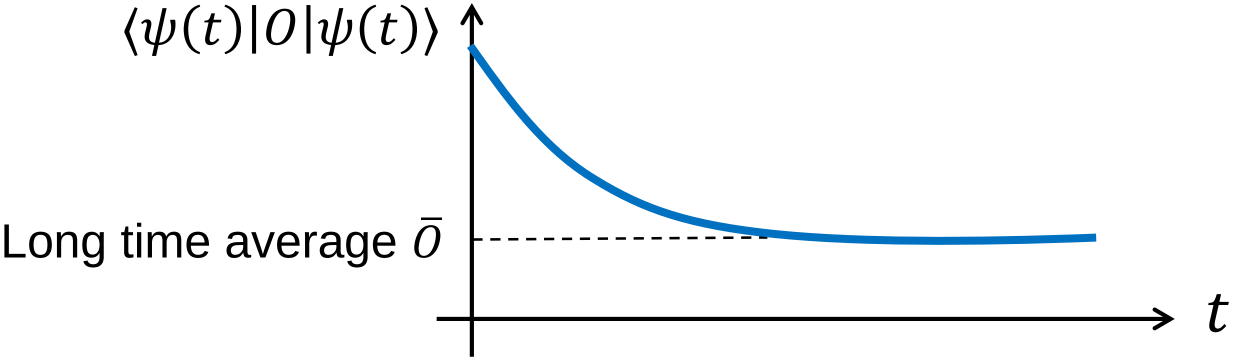
Bloch group, Nature physics (2012)

Superconducting qubits



Martinis group, Nature Physics (2016)

# Quantum ergodicity



A pure state can reach thermal equilibrium after (reasonable) relaxation time by unitary dynamics

*When* and *why* $\bar{O} \simeq \mathrm{tr}[O\rho_{\mathrm{MC}}]$ ?

$\uparrow$ **Long-time average**

$\uparrow$ **Microcanonical average**

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# Eigenstate-thermalization hypothesis (ETH)

Srednicki, PRE **50**, 888 (1994); Rigol, Dunjko, Olshanii, Nature **452**, 854 (2008)

***All*** the energy eigenstates are thermal

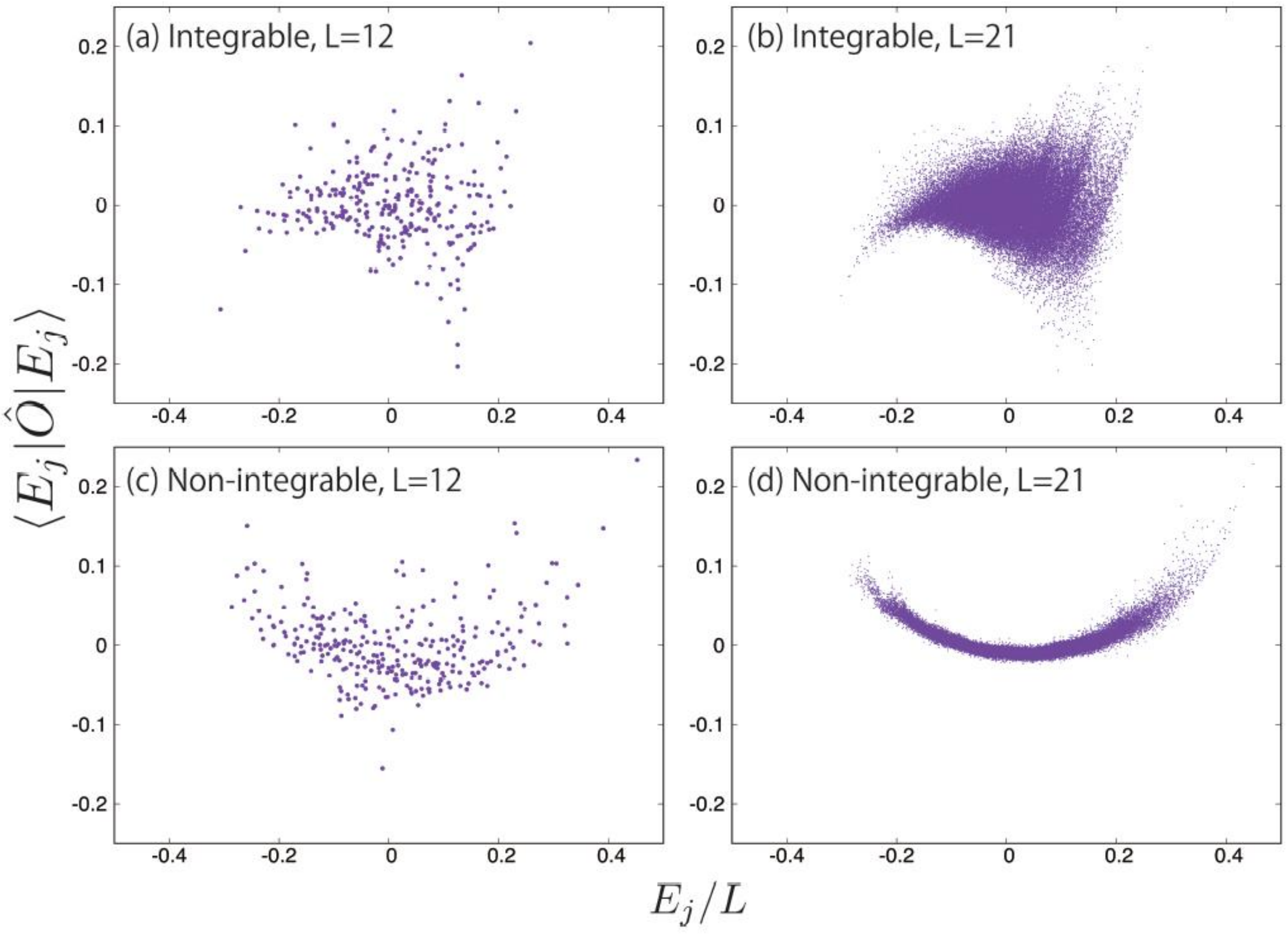
$$\langle E_i|O|E_i\rangle \simeq \mathrm{tr}[O\rho_{\mathrm{MC}}]$$

Microcanonical average

Believed to be true (from numerical evidences)
only for non-integrable systems under reasonable assumptions
(e.g., local interaction, translation invariance,…)

**Sufficient condition for thermalization!**

$$\text{Long time average} = \sum_i |c_i|^2 \langle E_i|O|E_i\rangle \simeq \mathrm{tr}[O\rho_{\mathrm{MC}}]$$



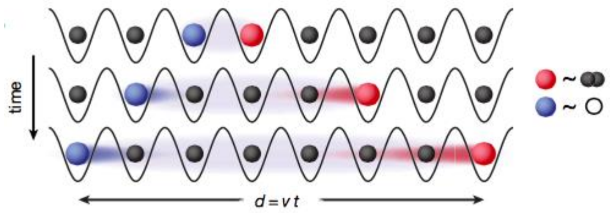
Integrable: XXZ, Non-integrable: XXZ +nnn

K. Kaneko, E. Iyoda, T. Sagawa, Bulletin of Physical Society of Japan (2018)

# Lattice systems

A good platform to study quantum many-body systems

- ✓ Fundamental theorems have been rigorously established
- ✓ Various numerical studies
- ✓ Experimentally accessible with ultracold atoms



M. Cheneau *et al.*, Nature 481, 484 (2012)

Especially, we focus on situations where:

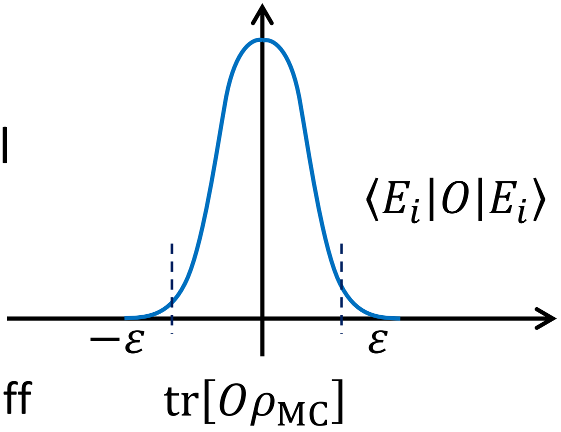
- $d$-dim, periodic boundary
- Local interaction
- Translation invariant ⇒ *No localization*
- Exponential decay of correlation functions ⇒ *Not on a critical point*

$N$: the system size (the number of the lattice sites)
$D$: the dimension of the microcanonical energy shell

Boltzmann entropy: $S = k_{\mathrm{B}} \ln D$

# Formalize ETHs

**Strong ETH:** *All* the energy eigenstates are thermal
**Weak ETH:** *Almost all* the energy eigenstates are thermal



Let $O$ an observable with $\|O\| = 1$. Let $\varepsilon > 0$.

An energy eigenstate $|E_i\rangle$ is called $\varepsilon$-*thermal* with respect to $O$ iff

$$|\mathrm{tr}[O\rho_{\mathrm{MC}}] - \langle E_i|O|E_i\rangle| < \varepsilon.$$

Let $D_{\mathrm{out}}^{\varepsilon}$ be the number of eigenstates $|E_i\rangle$ that are not $\varepsilon$-thermal.

Now define:

- $(H, O)$ satisfies **the strong ETH**, iff
  for any $\varepsilon > 0$, there exists $N_0$ such that for all $N \geq N_0$, $D_{\mathrm{out}}^{\varepsilon} = 0$.

- $(H, O)$ satisfies **the weak ETH**, iff for any $\varepsilon > 0$, $\lim_{N\to\infty} \frac{D_{\mathrm{out}}^{\varepsilon}}{D} = 0$.

Rem. If the Hamiltonian has degeneracy, we should add “there exists an energy eigenbasis…”

# Validity of ETH

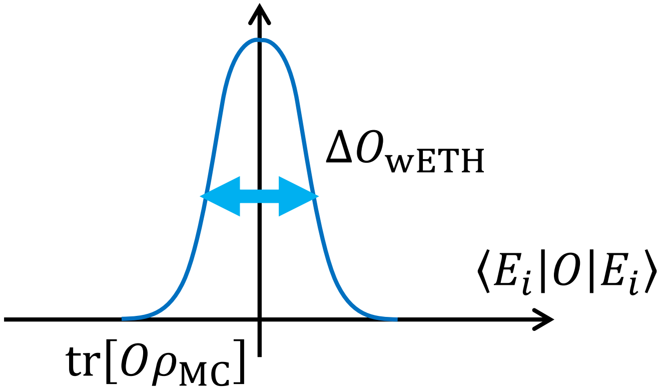
| | Thermalization to microcanonical | Strong ETH | Weak ETH |
|---|---|---|---|
| Nonintegrable | ○ | ○ | ○ |
| Integrable | × | × | ○ |
| Localized | × | × | × |

Integrable system does not thermalize:

**Strong ETH is the plausible scenario of thermalization!**

# Weak ETH: Variance

$O$: quasi-local observable with $\|O\| = 1$,
Size of its support: $|\mathrm{supp} O| = \mathcal{O}(N^{\alpha})$, $0 \leq \alpha < 1/2$



**Fluctuation over energy eigenstates:**

$$(\Delta O_{\mathrm{wETH}})^2 := \frac{1}{D}\sum_{i\in M}(\langle E_i|O|E_i\rangle - \mathrm{tr}[O\rho_{\mathrm{MC}}])^2$$

**Make some additional assumptions:**

that are needed for the local equivalence of ensembles:

- ✓ Exponential decay of correlations ⇒ *Not on a critical point*
- ✓ Rapid convergence of the free energy

**Our theorem:** Iyoda, Kaneko, Sagawa, Phys. Rev. Lett. **119**, 100601 (2017)

$$(\Delta O_{\mathrm{wETH}})^2 \leq \mathcal{O}(N^{-\frac{(1-2\alpha)}{4}+\delta})$$

$\delta > 0$: can be arbitrarily small

The case of $\alpha = 0$ was discussed by Biroli, Kollath, Läuchli, PRL **105**, 250401 (2010)
(But their proof was not rigorous. Our proof is based on the local equivalence of ensembles by Tasaki, arXiv:1609.0698)

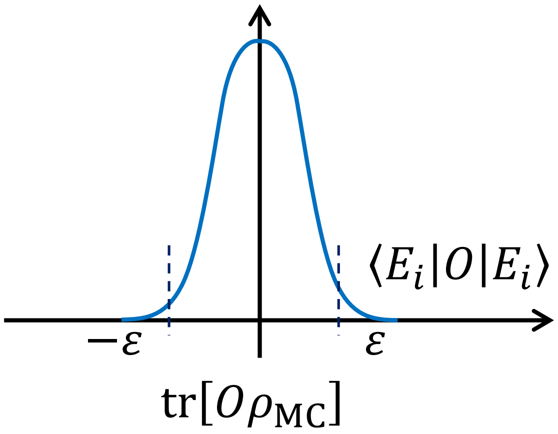
**In reality (numerics):**

**Integrable:** $(\Delta O_{\mathrm{wETH}})^2 = O(N^{-1})$, **Non-integrable:** Essentially, $(\Delta O_{\mathrm{wETH}})^2 = e^{-O(N)}$

# Weak ETH: Large deviation

$O$: **local** observable with $\|O\| = 1$

$D$: dimension of the microcanonical energy shell
$D_{\mathrm{out}}^{\varepsilon}$ : the number of athermal eigenstates
$N$: the number of lattice sites



$$\frac{D_{\mathrm{out}}^{\varepsilon}}{D} \leq \exp(-\gamma_{\varepsilon} N + o(N))$$

$\gamma_{\varepsilon} > 0, \gamma_{\varepsilon} = \mathcal{O}(\varepsilon^2)$

**This is rigorous and applicable to both integrable and non-integrable cases**

Under the assumptions of translation invariance, not on a critical point, etc

But this theorem does **not** guarantee the strong ETH,
because $D_{\mathrm{out}}^{\varepsilon}$ itself can be exponentially large (as $D$ is exponentially large)

K. Netocny, F. Redig, J. Stat. Phys. **117**, 521 (2004).
M. Lenci, L. Rey-Bellet, J. Stat. Phys. **119**, 715 (2005).
Y. Ogata, Comm. Math. Phys. **296**, 35 (2010).

H. Tasaki, J. Stat. Phys. **163**, 937 (2016).
T. Mori, arXiv:1609.09776 (2016) .

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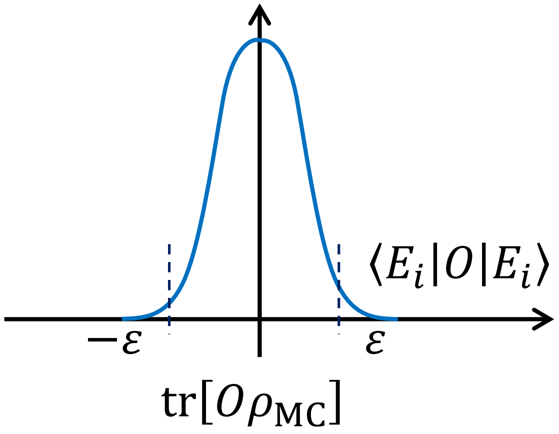
# Numerical large deviation analysis

T. Yoshizawa, E. Iyoda, T. Sagawa,
PRL **120**, 200604 (2018).



Slightly modified definition of athermal eigenstates:

Let $D_{\mathrm{out}}$ be the number of eigenstates $i \in M(E,\Delta)$ that are not thermal in the following sense:

$$|\mathrm{tr}[O\rho_{\mathrm{MC}}(E_i,\delta)] - \langle E_i|O|E_i\rangle| > \varepsilon$$

$$\Delta = \mathcal{O}(N), \delta = \mathcal{O}(1)$$

Cf. The previous (standard) definition:

$$|\mathrm{tr}[O\rho_{\mathrm{MC}}(E,\Delta)] - \langle E_i|O|E_i\rangle| > \varepsilon,\ \mathcal{O}(1) \leq \Delta \leq \mathcal{O}(\sqrt{N})$$

# Numerical large deviation analysis: **Integrable**

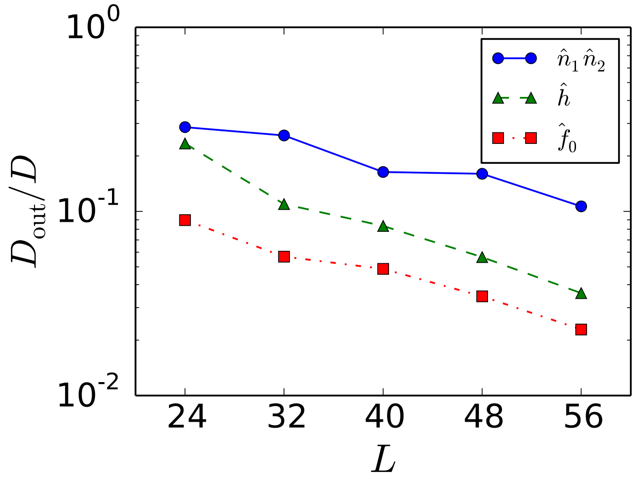
T. Yoshizawa, E. Iyoda, T. Sagawa, PRL **120**, 200604 (2018).

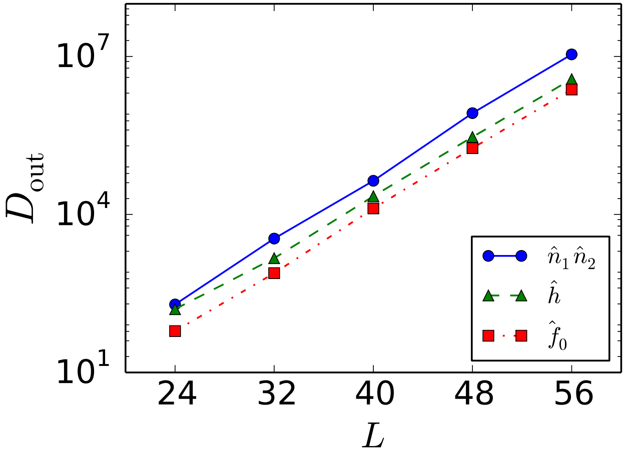
1d spin chain (= hardcore bosons)

$$\left[\hat{b}_i^\dagger, \hat{b}_j\right] = \left[\hat{b}_i, \hat{b}_j\right] = \left[\hat{b}_i^\dagger, \hat{b}_j^\dagger\right] = 0 \quad \left\{\hat{b}_i^\dagger, \hat{b}_i\right\} = 1, \left\{\hat{b}_i, \hat{b}_i\right\} = \left\{\hat{b}_i^\dagger, \hat{b}_i^\dagger\right\} = 0$$

**Integrable case: XX model**

$$\hat{\mathcal{H}}_{XX} := -\sum_{i=1}^{L}\left[\hat{b}_i^\dagger \hat{b}_{i+1} + h.c.\right]$$





$$\hat{n}_1\hat{n}_2 = \hat{b}_1^\dagger\hat{b}_1\hat{b}_2^\dagger\hat{b}_2$$

$$\hat{h} = \frac{1}{L}\sum_i\left[\hat{b}_i^\dagger\hat{b}_{i+3} + h.c.\right]$$

$$\hat{f}_0 = \frac{1}{L}\sum_{ij}\hat{b}_i^\dagger\hat{b}_j$$

Exponential decay of $D_{\mathrm{out}}/D$ ➡ Strong ETH is false

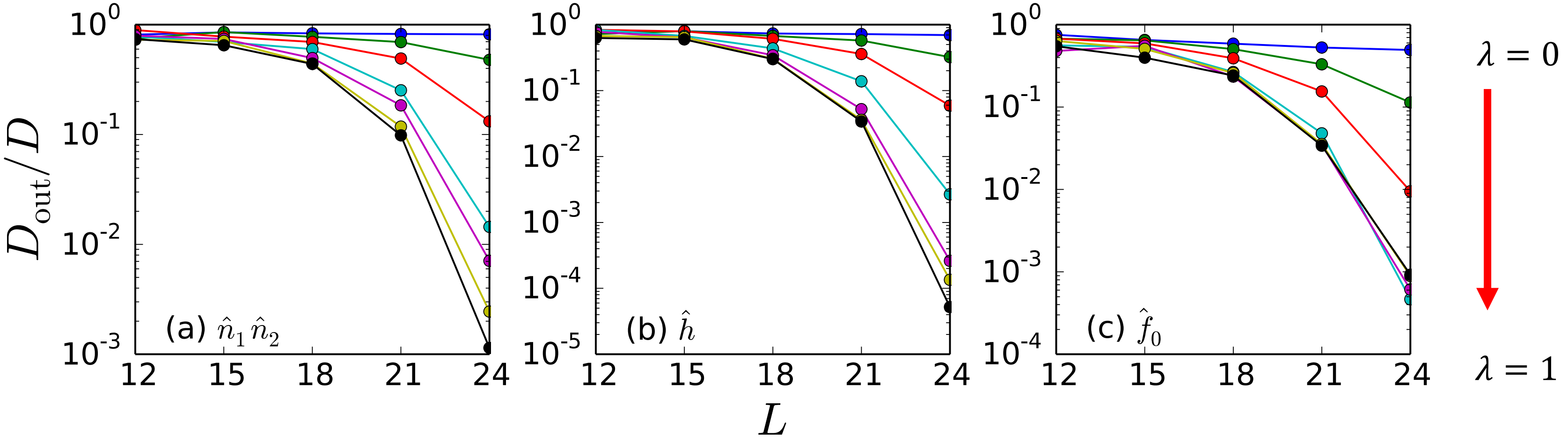
# Numerical large deviation analysis: **Non-integrable**

T. Yoshizawa, E. Iyoda, T. Sagawa, PRL **120**, 200604 (2018).

**Nonintegrable case: XXX +nnn** $\hat{\mathcal{H}}_{XXX} := \frac{1}{1+\lambda}\left[\hat{\mathcal{H}}_0 + \lambda \hat{W}\right]$

$\hat{\mathcal{H}}_0$ : XXX Hamiltonian $\hat{W}$ : next-nearest term

$\lambda$ : intergrability-breaking parameter

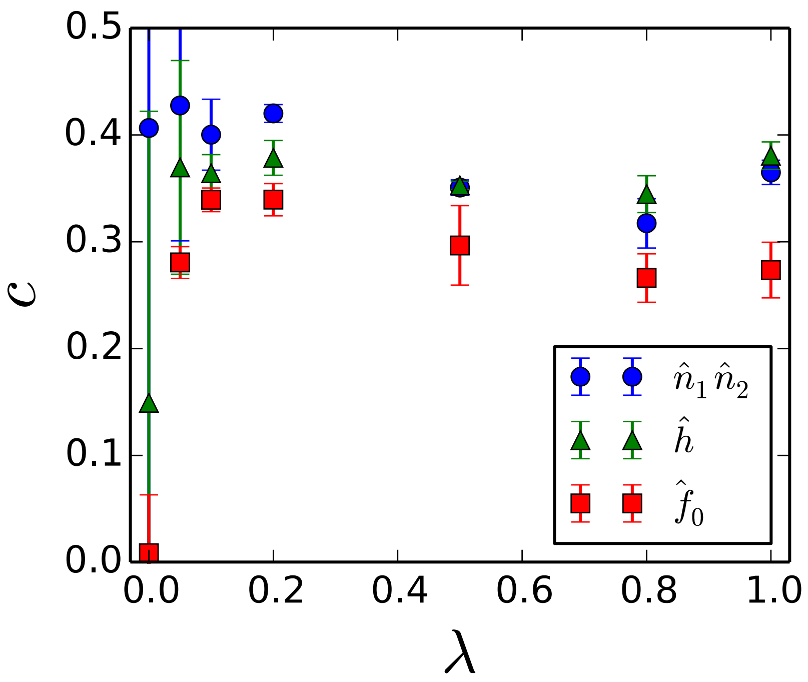


**Double exponential** decay of $D_{\mathrm{out}}/D$ ➡ Strong ETH is true (even **near integrability**!)

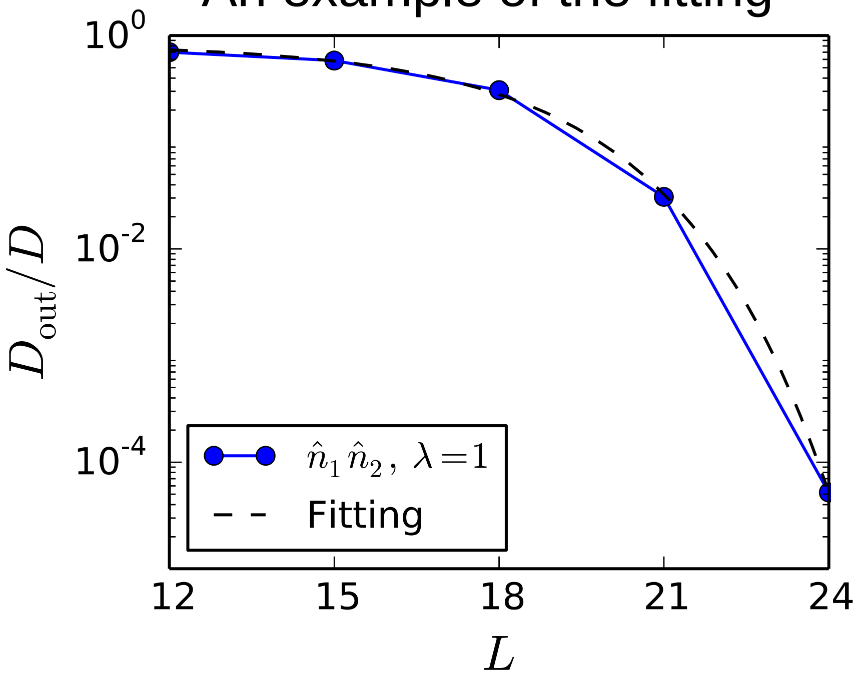
# Double exponential decay of $D_{\mathrm{out}}/D$

T. Yoshizawa, E. Iyoda, T. Sagawa, PRL **120**, 200604 (2018).

$$f(L) := a \exp\left(-b \exp(cL)\right)$$



An example of the fitting



Consistent with random matrix theory

# Validity of ETH

| | Thermalization to microcanonical | Strong ETH | Weak ETH |
|---|---|---|---|
| Nonintegrable | ○ | ○ | ○ |
| Integrable | × | × | ○ |
| Localized | × | × | × |

Integrable system does not thermalize:
**Strong ETH is the plausible scenario of thermalization!**

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# Second law and fluctuation theorem

**Second law** Entropy production is non-negative on average

$$\langle \sigma \rangle \geq 0$$

**Fluctuation theorem** Universal relation far from equilibrium

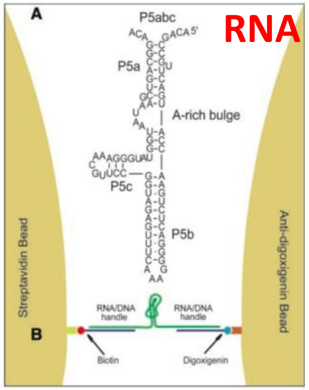
$$\langle e^{-\sigma} \rangle = 1$$

Second law as an **equality**!

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

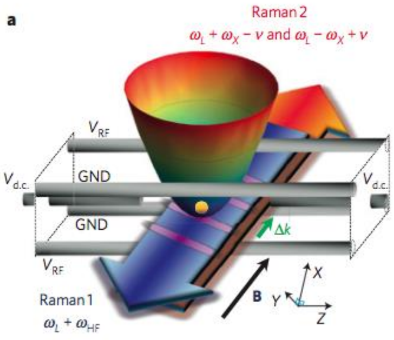
Experiment（2000’s-）
Colloidal particle, Biomolecule,
Single electron, Ion trap, NMR, …

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, …

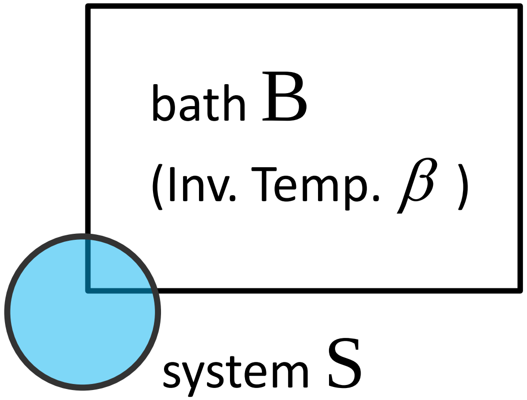
Total system: system S and bath B

(arbitrary: **Not** necessarily on a lattice!)

**S+B obeys unitary dynamics**

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

$$\hat{H}=\hat{H}_{\mathrm{S}}+\hat{H}_{\mathrm{I}}+\hat{H}_{\mathrm{B}}$$



- Initial state of S: arbitrary
- **Initial state of B: Canonical**

  **→ This is a very special assumption that leads to the second law.**
- No initial correlation between S and B.

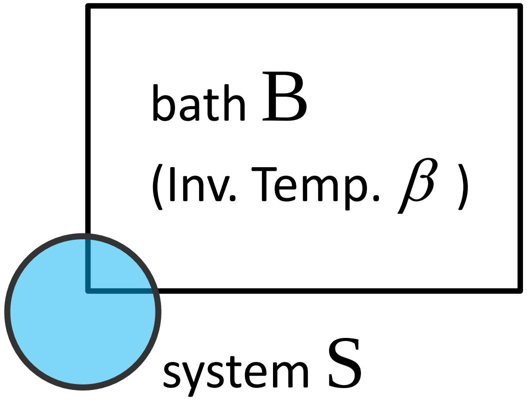
$$\hat{\rho}(0)=\hat{\rho}_{\mathrm{S}}(0)\otimes\hat{\rho}_{\mathrm{B}}(0),\quad \hat{\rho}_{\mathrm{B}}(0)=e^{-\beta\hat{H}_B}/Z_B$$

# Second law (Clausius inequality)

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

**von Neumann entropy**

**Heat**



bath $\mathrm{B}$

(Inv. Temp. $\beta$ )

system $\mathrm{S}$

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

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

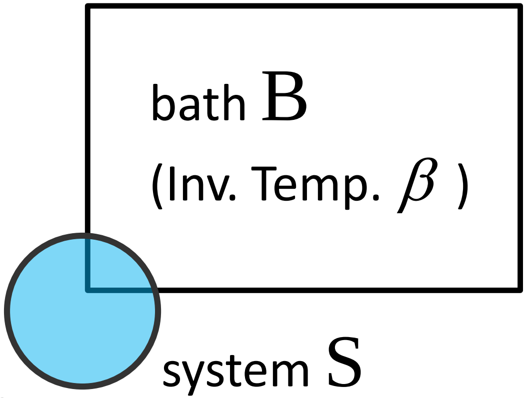
**Information entropy** and **Heat** are linked!

(if the initial state of bath $\mathrm{B}$ is **canonical**)

$$\langle\sigma\rangle \equiv \Delta S_\mathrm{S} - \beta\langle Q\rangle \geq 0$$

: entropy production on average
(non-negative)

# Fluctuation theorem



bath $\mathrm{B}$

(Inv. Temp. $\beta$ )

system $\mathrm{S}$

$\sigma$ : stochastic entropy production (fluctuates)

Let $\hat{\sigma}(t) \equiv -\ln \hat{\rho}_{\mathrm{S}}(t) + \beta \hat{H}_B$

Projection measurements of $\hat{\sigma}(t)$at initial and final times
Difference of outcomes: $\sigma$

**Integral fluctuation theorem** (Jarzynski equality)

$$\boxed{\left\langle e^{-\sigma} \right\rangle = 1}$$

Second law can be expressed by an **equality** with full cumulants (even if $\mathrm{S}$ is far from equilibrium)

Reproduces the second law by $\left\langle e^{-\sigma} \right\rangle \geq e^{-\langle \sigma \rangle}$

and the fluctuation-dissipation theorem, etc.

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# Second law for a single energy eigenstate?

Conventional derivation of the second law:
The initial canonical distribution of the bath ⇒ The second law

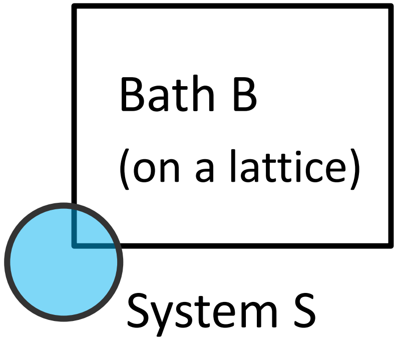
ETH argument:
Even a single energy eigenstate can be thermal;
The canonical distribution is just a statistical-mechanical *ansatz* to compute thermodynamic quantities in equilibrium.

Question:
Is it possible to prove the second law when the initial state of the bath is a single energy eigenstate, as a theorem of quantum mechanics?

**Our theorem (roughly):**

$\Delta S_S - \beta Q \geq -\varepsilon$ holds for most of the energy eigenstates

# Setup



- Small system S is locally in contact with a large bath B: $H = H_\mathrm{S} + H_\mathrm{I} + H_\mathrm{B}$

- Initial state: $\rho(0) = \rho_\mathrm{S}(0) \otimes |E_i\rangle\langle E_i|$

  $\rho_\mathrm{S}(0)$ is arbitrary, $|E_i\rangle$ is a **thermal** eigenstate

- B is on a lattice and satisfies some assumptions required for the ETH and the "Lieb-Robinson bound." Especially:
  - Local interaction
  - Translation invariant ⇒ *No localization*
  - Exponential decay of correlations ⇒ *Not on a critical point*

# Second law (Clausius inequality)

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

$\varepsilon$ **: Small error term**

For any $\varepsilon > 0$, for any $t$, there exists a sufficiently large bath, such that...

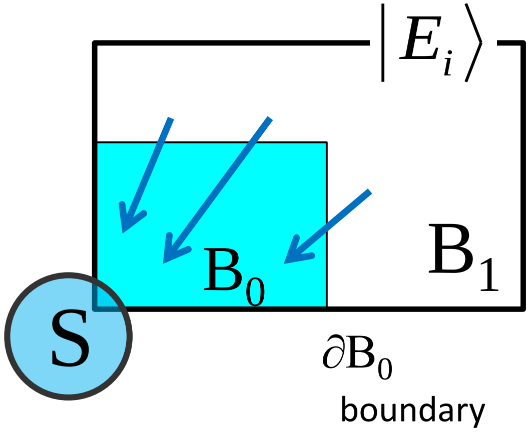
→ **Mathematically rigorous**

**Even though the state of $\mathrm{B}$ is an energy eigenstate, information and thermodynamics are linked**

Size of the bath: $N = O(\varepsilon^{-4(1-2\alpha)-\delta})$

Lieb-Robinson time: $\tau = O(N^{\alpha/d})$ $\quad 0 < \alpha < 1/2 \quad \delta = +0$

# Key of the proof: Lieb-Robinson bound



**The velocity of “information propagation” in $\mathrm{B}$ is finite, due to locality of interaction**

Effective **“light-cone”** like structure

⇒ $\mathrm{S}$ is not affected by $\mathrm{B}_1$ in the short time regime

⇒ $\mathrm{S}$ feels as if $\mathrm{B}$ is in the canonical distribution if the initial energy eigenstate of $\mathrm{B}$ satisfies ETH

## Lieb-Robinson bound

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

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

$v/\mu$ : Lieb-Robinson velocity

$\tau$ : **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)

# Integral fluctuation theorem

$$\left| \langle e^{-\sigma} \rangle - 1 \right| \leq \varepsilon$$

For any $\varepsilon > 0$, 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**

Size of the bath: $N = O(\varepsilon^{-4(1-2\alpha)-\delta})$

Lieb-Robinson time: $\tau = O(N^{\alpha/d})$ $0 < \alpha < 1/2$ $\delta = +0$

# Numerical simulation: Setup

Hard core bosons with nearest-neighbor repulsion (equivalent to XXZ)

$$\{\hat{c}_i, \hat{c}_i^{\dagger}\} = 1, \ \ \{\hat{c}_i, \hat{c}_i\} = \{\hat{c}_i^{\dagger}, \hat{c}_i^{\dagger}\} = 0 \qquad [\hat{c}_i, \hat{c}_j^{\dagger}] = [\hat{c}_i, \hat{c}_j] = [\hat{c}_i^{\dagger}, \hat{c}_j^{\dagger}] = 0 \ \ \text{for } i \neq j$$

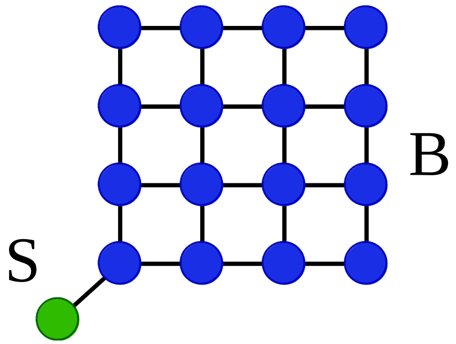
$$\hat{H}_{\mathrm{S}} = \varepsilon \hat{c}_0^{\dagger} \hat{c}_0 \qquad \hat{H}_{\mathrm{I}} = -\gamma' \sum_{\langle 0, j \rangle} \left( \hat{c}^{\dagger}{}_0 \, \hat{c}_j + \hat{c}^{\dagger}{}_j \, \hat{c}_0 \right)$$

$$\hat{H}_{\mathrm{B}} = \varepsilon \sum_{i} \hat{c}_i^{\dagger} \hat{c}_i - \gamma \sum_{\langle i, j \rangle} \left( \hat{c}^{\dagger}{}_i \, \hat{c}_j + \hat{c}^{\dagger}{}_j \, \hat{c}_i \right) + g \sum_{\langle i, j \rangle} \hat{c}^{\dagger}{}_i \, \hat{c}_i \hat{c}^{\dagger}{}_j \, \hat{c}_j$$

$\gamma / \varepsilon = 1, \ \ g / \varepsilon = 0.1$

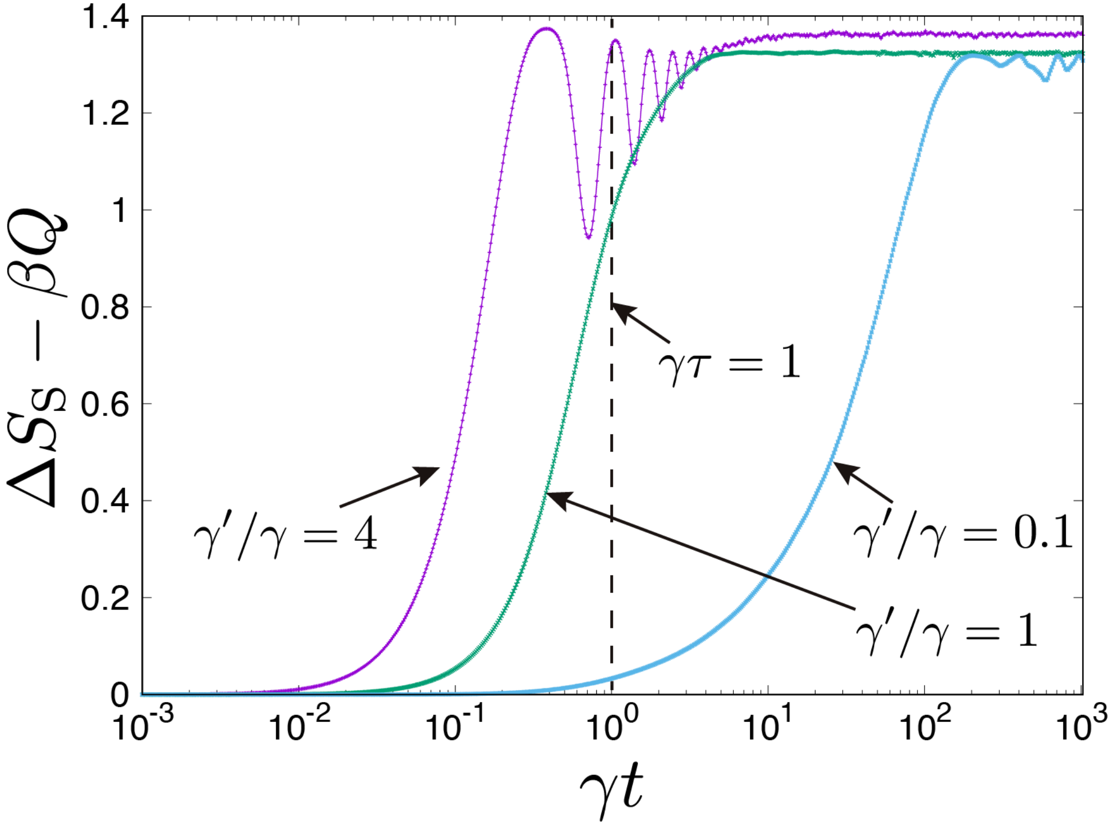
Initial state: $\hat{\rho}_{\mathrm{S}}(0) = |1\rangle\langle 1|$

Bath: 4 bosons, $\beta = 0.1$



**Method: Exact diagonalization (full)**

# Second law



Lieb-Robinson Time

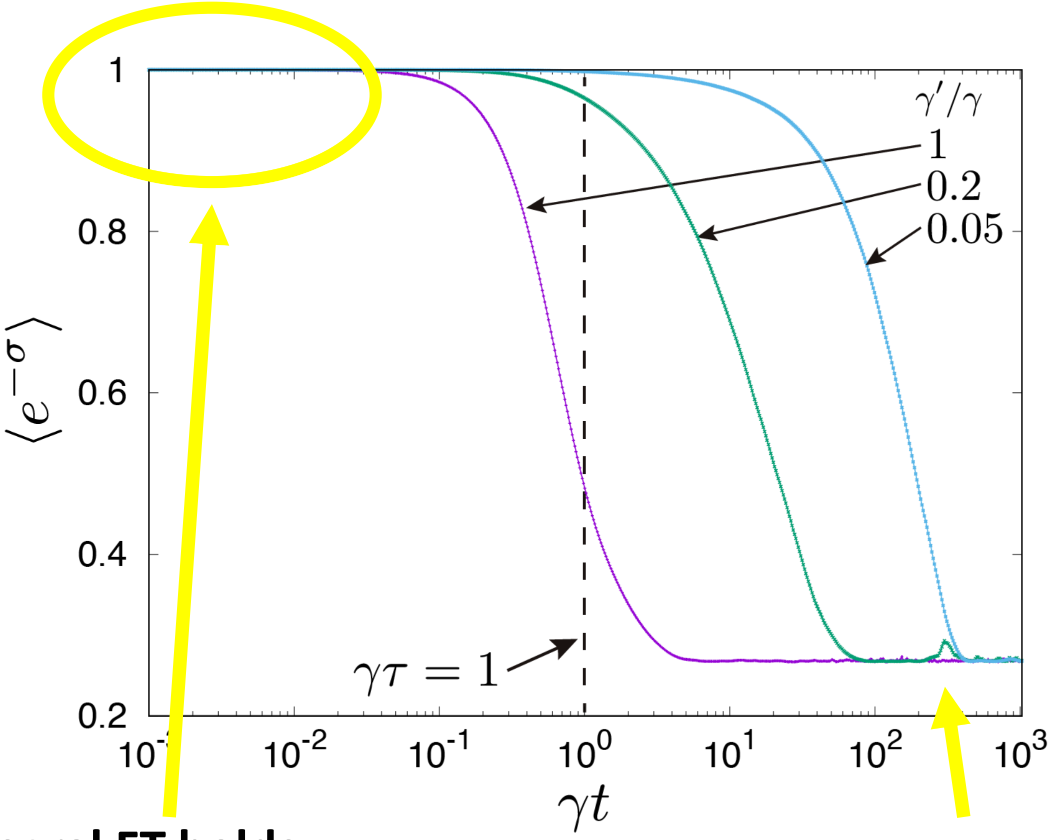
$\tau \sim 1/\gamma$

Average entropy production is always non-negative

Even beyond the Lieb-Robinson time

→ Kaneko, Iyoda, Sagawa, Phys. Rev. E **96**, 062148 (2017).

# Integral fluctuation theorem



Lieb-

Robinson

Time

$\tau \sim 1/\gamma$

**Integral FT holds**
(But quite subtle, because of the large finite-size effect)

**Deviation comes from “bare” quantum fluctuation**

**Dynamical crossover** from thermal fluctuation to bare quantum fluctuation

# Estimation of the LR time $\tau$

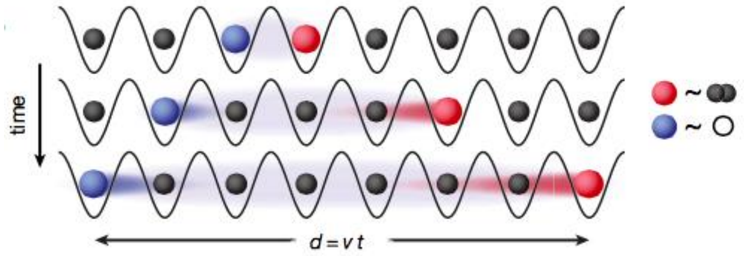
**Coffee in a room:** $\tau \sim$ms very short!

**If** air of the room was in an energy eigenstate,
then the FT would hold only in such a short time scale.

**Ultracold atoms:** $\tau \sim L^{1/2}\hbar/J$

Can be hundreds times of the
experimental time scale $\hbar/J$

$J$: tunneling amplitude
$L$: the side length (the number of the sites) of the system

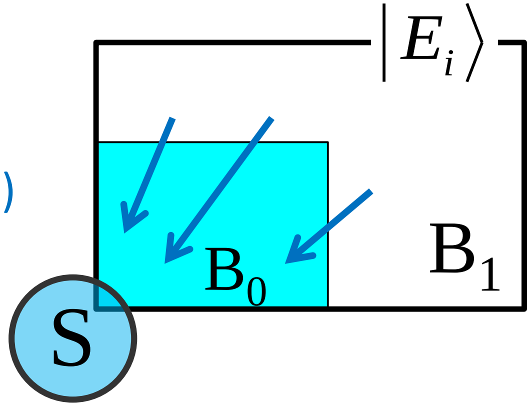


M. Cheneau *et al.*, Nature 481, 484 (2012)

Clear verification of the FT would be possible

# Summary

E. Iyoda, K. Kaneko, T. Sagawa,
Phys. Rev. Lett. **119**, 100601 (2017)



**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

  **Both in the short and long time regimes**

- ✓ **Fluctuation theorem** $$\left|\left\langle e^{-\sigma}\right\rangle - 1\right| \leq \varepsilon_{\mathrm{FT}}$$

  Fundamental property of entropy production far from equilibrium

  **Only in the short time regime**

**Key ideas: ETH and Lieb-Robinson bound**

# Outline

- Introduction
- Eigenstate thermalization hypothesis (ETH)
  - Review of ETH
  - Our result: Numerical large deviation analysis
- Second law and fluctuation theorem
  - Conventional setup
  - Our result: SL and FT for pure quantum states

**Thank you for your attention!**