Second law and eigenstate thermalization in isolated quantum many-body systems

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Osaka University, 29 January 2019.

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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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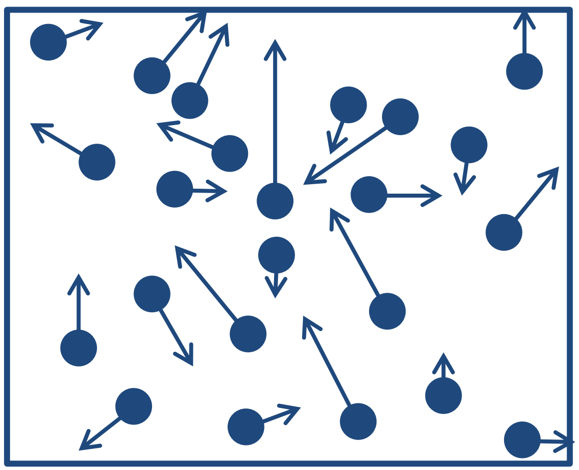
Origin of macroscopic irreversibility

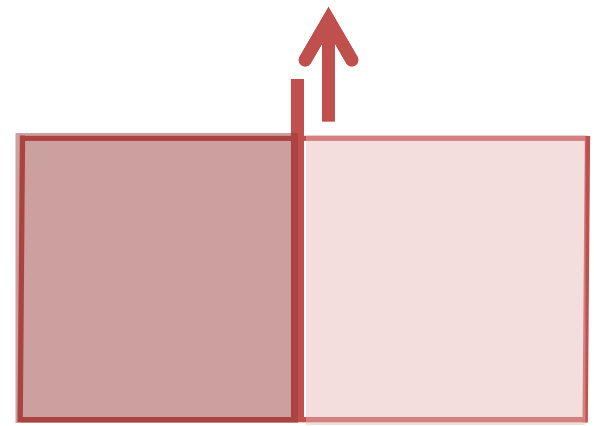
micro (Quantum mechanics)

reversible (unitary)

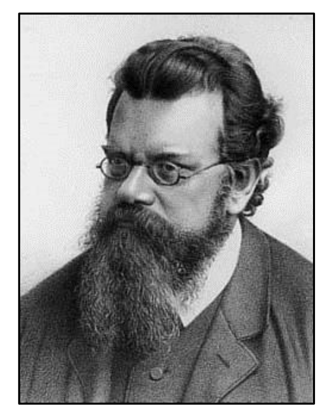


MACRO (Thermodynamics)

irreversible $\Delta S > 0$



Fundamental question since Boltzmann

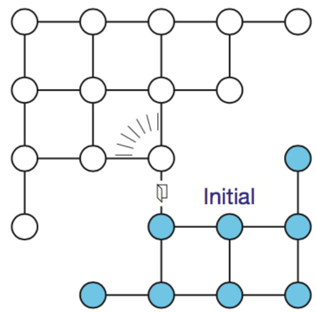


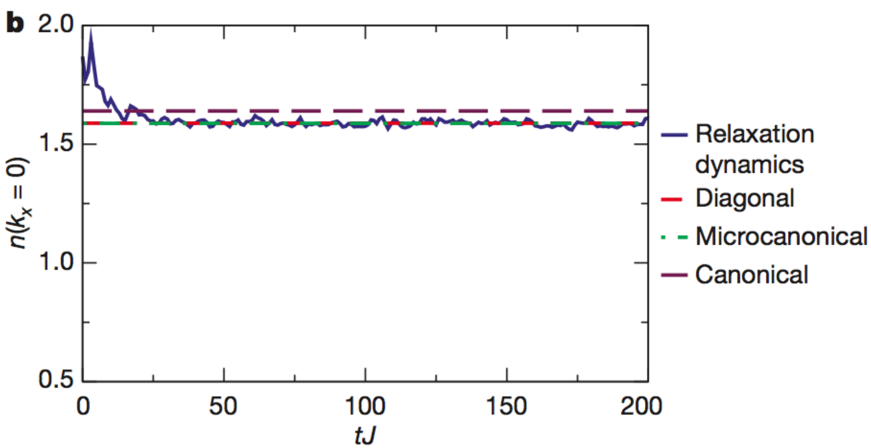
Modern progress

Numerical simulation:

Exact diagonalization

Hard-core bosons

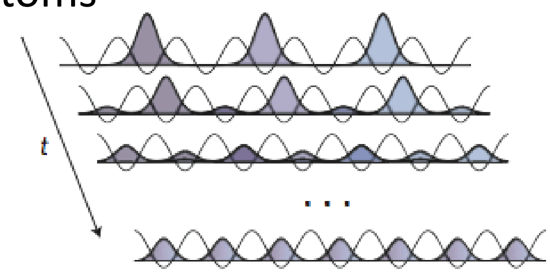




M. Rigol et al., Nature **452**, 854 (2008)

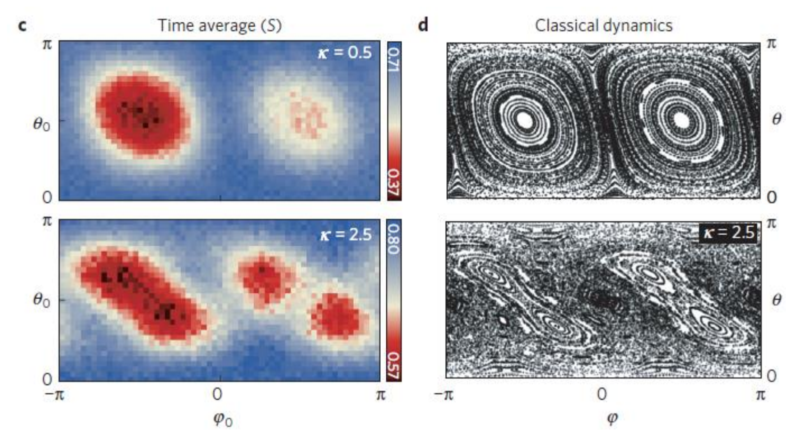
Experiments:

Ultracold atoms



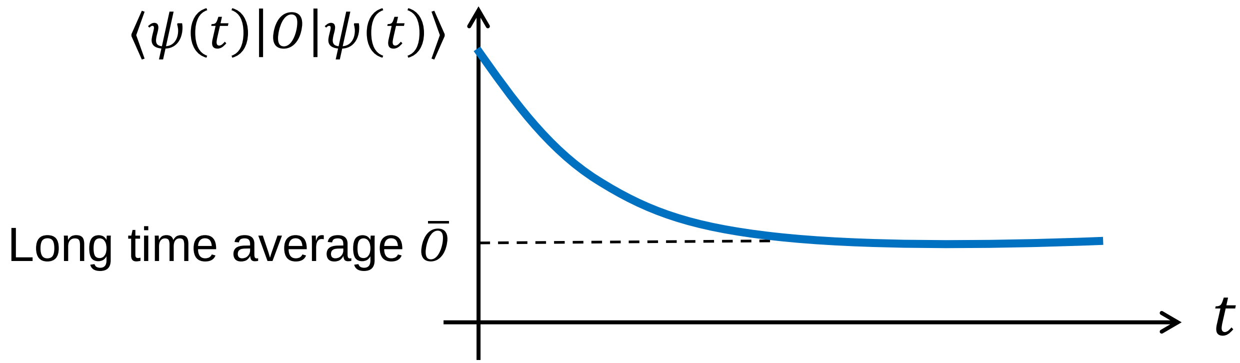
Bloch group, Nature physics (2012)

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

Long-time average

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

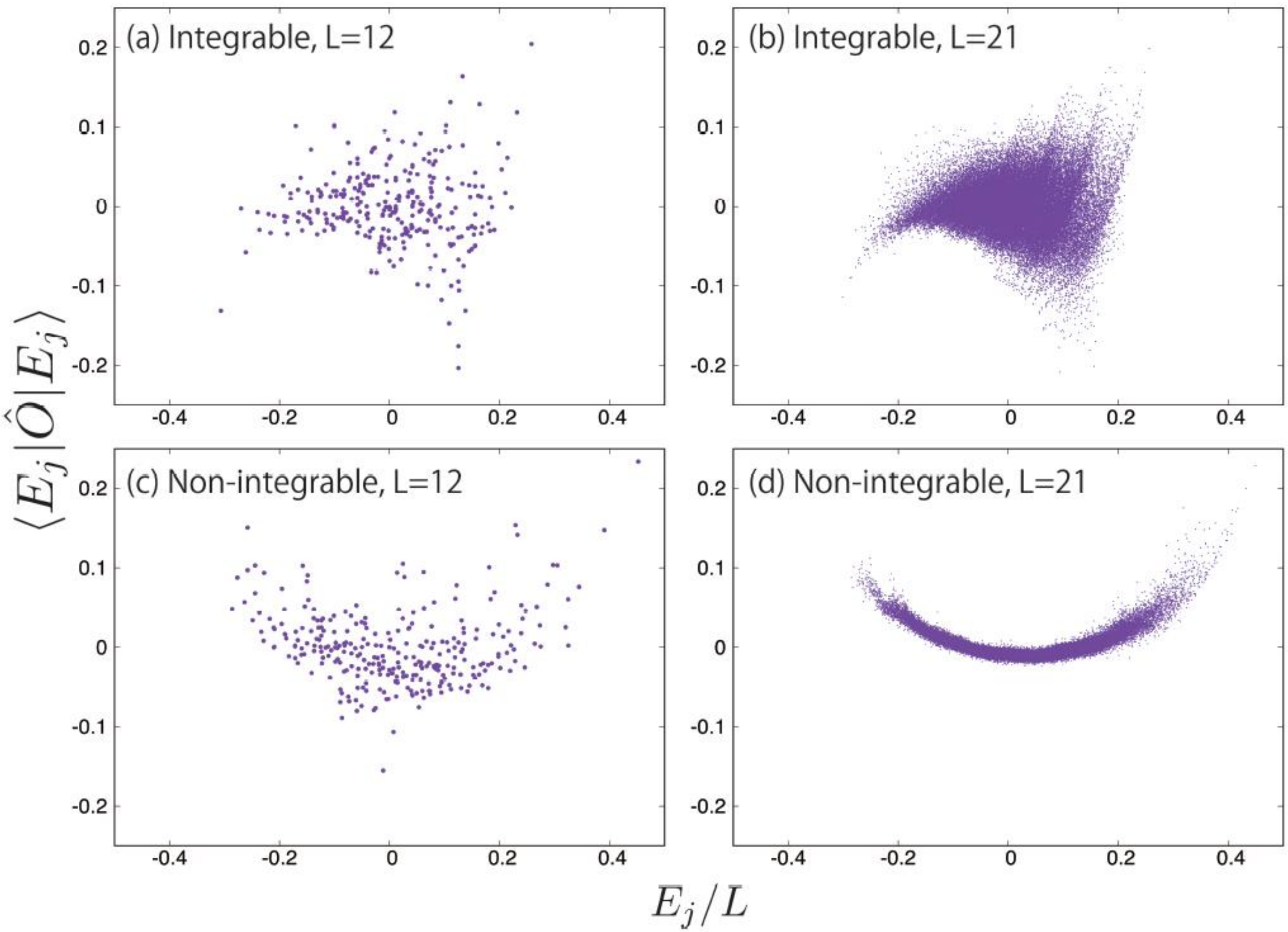
$$\langle E_i|O|E_i\rangle \simeq \mathrm{tr}[O\rho_{\mathrm{MC}}]$$

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!

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)

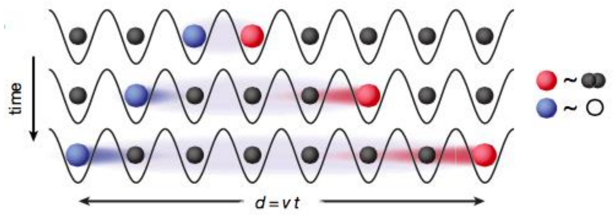
Lattice systems

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 $\Rightarrow$ *No localization*
- Exponential decay of correlation functions $\Rightarrow$ *Not on a critical point*

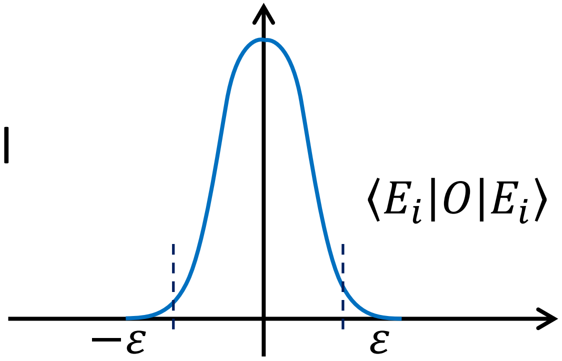
N: the system size (the number of the lattice sites)

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 ε-*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 ε-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…"

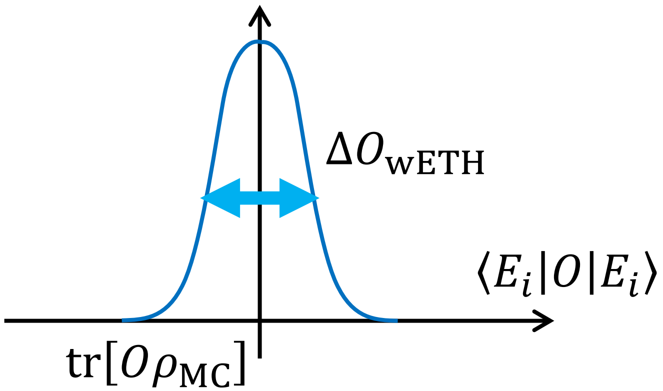
Validity of ETH

	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)

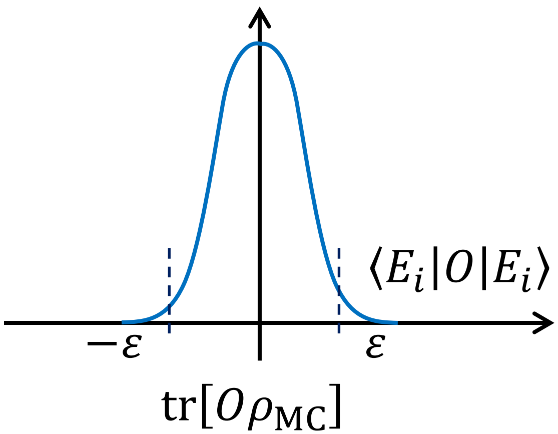
In reality (numerics):

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
$D_{\text{out}}^{\varepsilon}$: the number of athermal eigenstates
N: the number of lattice sites



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

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

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 $D_{\text{out}}^{\varepsilon}$ 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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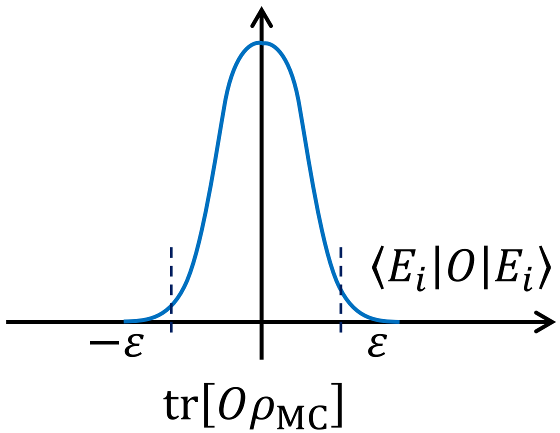
Numerical large deviation analysis

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



Slightly modified definition of
athermal eigenstates:

Let D_{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:

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

Numerical large deviation analysis: **Integrable**

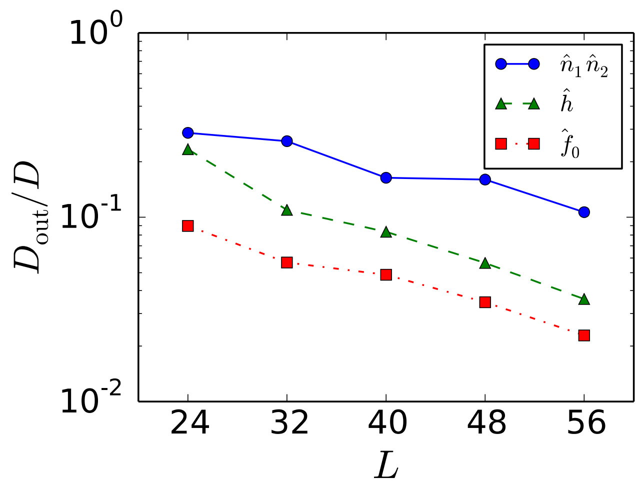
T. Yoshizawa, E. Iyoda, T. Sagawa, PRL **120**, 200604 (2018).

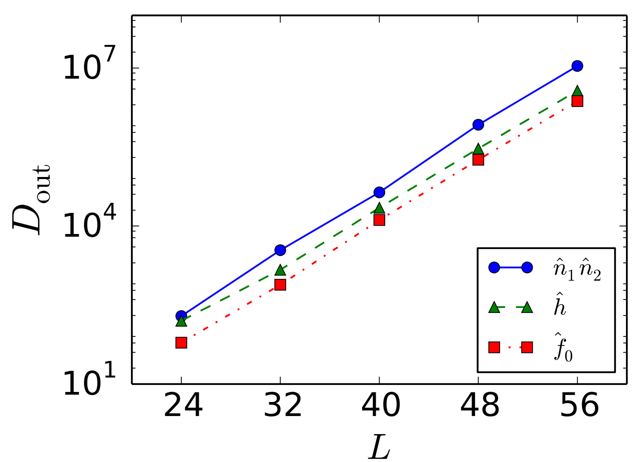
1d spin chain (= hardcore bosons)

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

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 $D_{\rm out}/D$ → Strong ETH is false

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

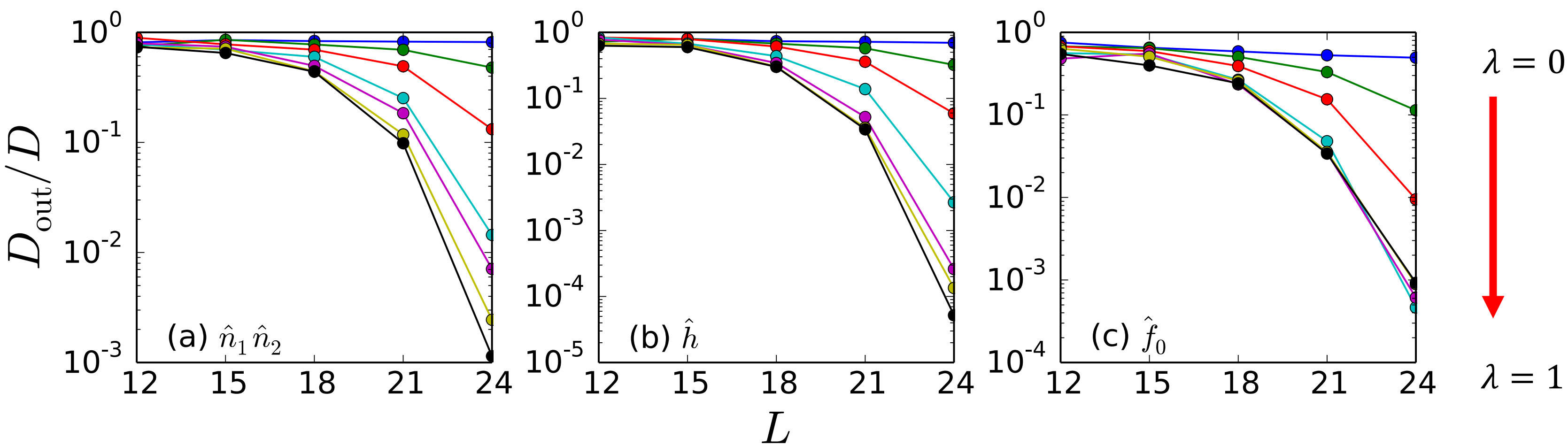
T. Yoshizawa, E. Iyoda, T. Sagawa, PRL **120**, 200604 (2018).

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

λ : intergrability-breaking parameter

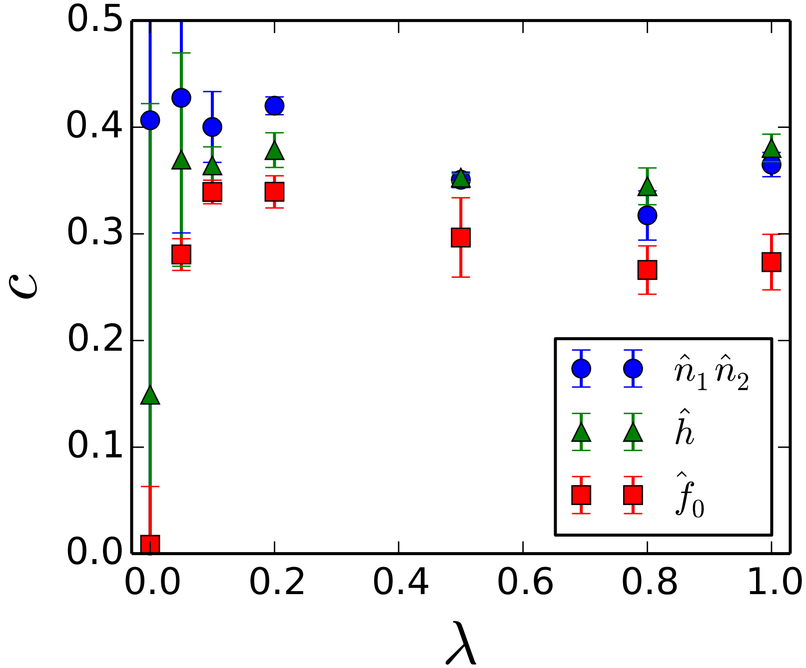


Double exponential decay of $D_{\rm out}/D$ ➡ Strong ETH is true (even **near integrability**!)

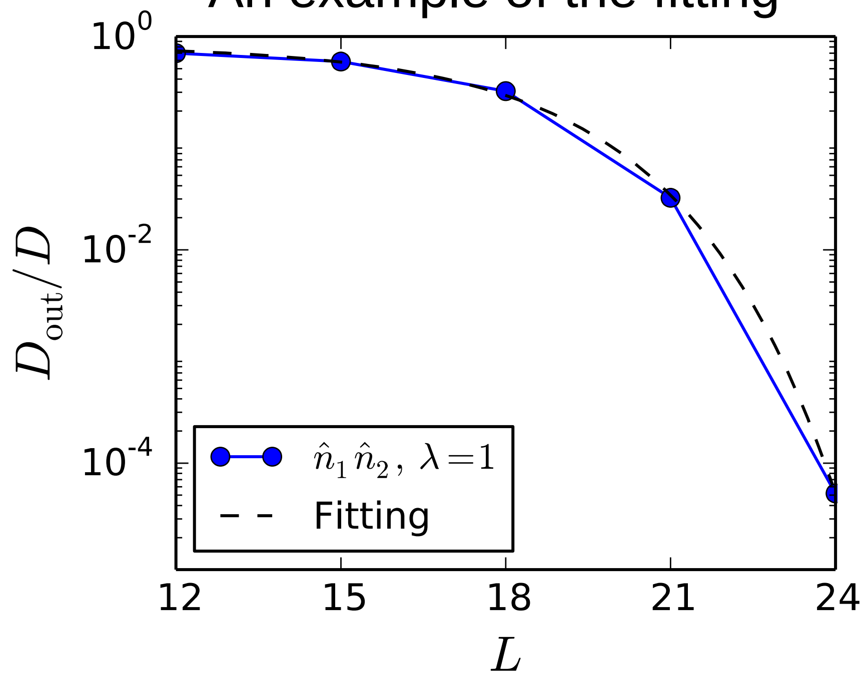
Double exponential decay of D_{out}/D

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

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



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

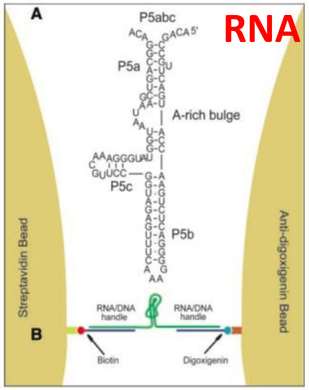
$$\left\langle e^{-\sigma} \right\rangle = 1$$

Second law as an **equality**!

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

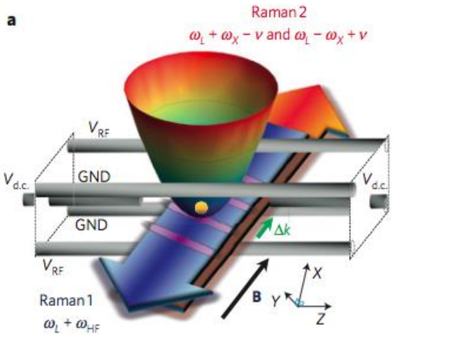
Experiment (2000's-)
Colloidal particle, Biomolecule,
Single electron, Ion trap, NMR, …

Classical



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

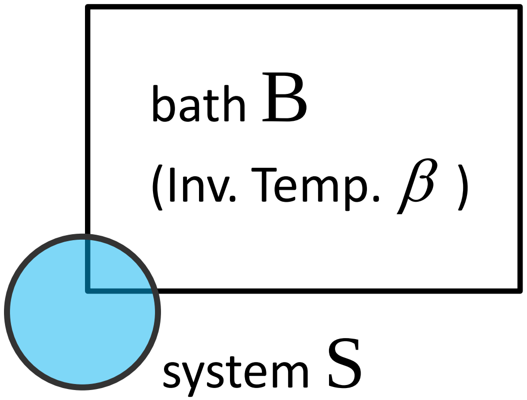
Quantum (Ion-trap)



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.

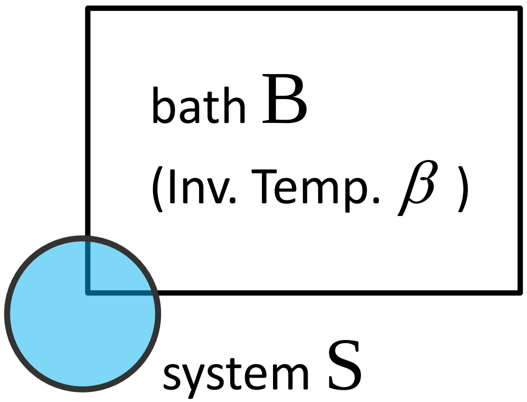
$$\hat{\rho}(0) = \hat{\rho}_{\mathrm{S}}(0) \otimes \hat{\rho}_{\mathrm{B}}(0), \quad \hat{\rho}_{\mathrm{B}}(0) = e^{-\beta \hat{H}_B} / Z_B$$

Second law (Clausius inequality)

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

von Neumann entropy

Heat



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

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

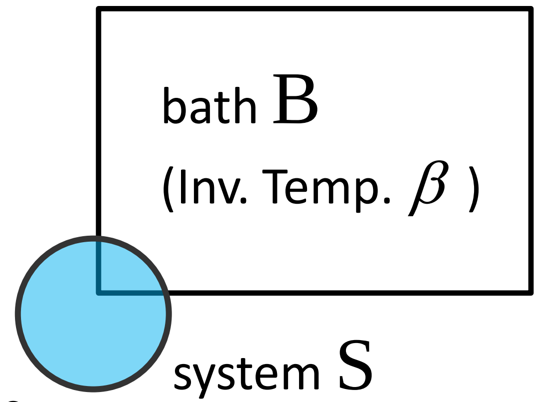
Information entropy and **Heat** are linked!

(if the initial state of bath 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



σ : 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: σ

Integral fluctuation theorem (Jarzynski equality)

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

Second law can be expressed by an **equality** with full cumulants (even if 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

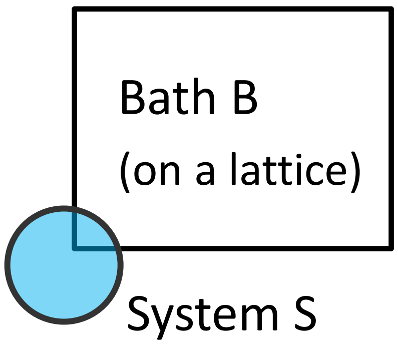
ETH argument:
Even a single energy eigenstate can be thermal;
The canonical distribution is just a statistical-mechanical *ansatz* to compute thermodynamic quantities in equilibrium.

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 $\Rightarrow$ *No localization*
  - Exponential decay of correlations $\Rightarrow$ *Not on a critical point*

Second law (Clausius inequality)

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

ε **: Small error term**

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

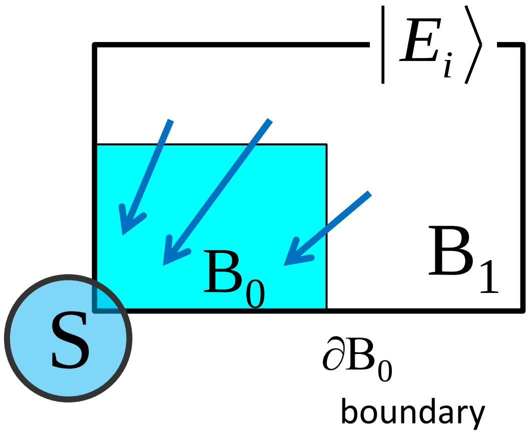
→ **Mathematically rigorous**

Even though the state of 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: $\tau = O(N^{\alpha/d})$ $0 < \alpha < 1/2$ $\delta = +0$

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 B_1 in the short time regime

S feels as if B is in the canonical distribution if the initial energy eigenstate of B satisfies ETH

Lieb-Robinson bound

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

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

v / μ : 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)

Integral fluctuation theorem

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

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

Numerical simulation: Setup

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

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

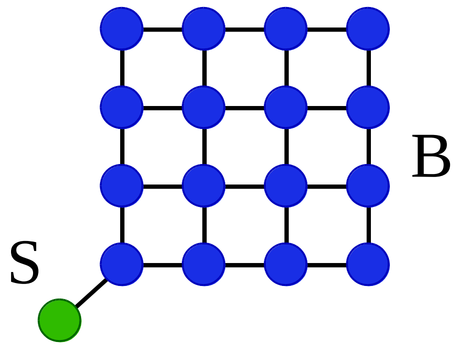
$$\hat{H}_{\mathrm{S}} = \varepsilon \hat{c}_0^{\dagger} \hat{c}_0 \qquad \hat{H}_{\mathrm{I}} = -\gamma' \sum_{\langle 0, j \rangle} \left(\hat{c}^{\dagger}{}_0 \, \hat{c}_j + \hat{c}^{\dagger}{}_j \, \hat{c}_0 \right)$$

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

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

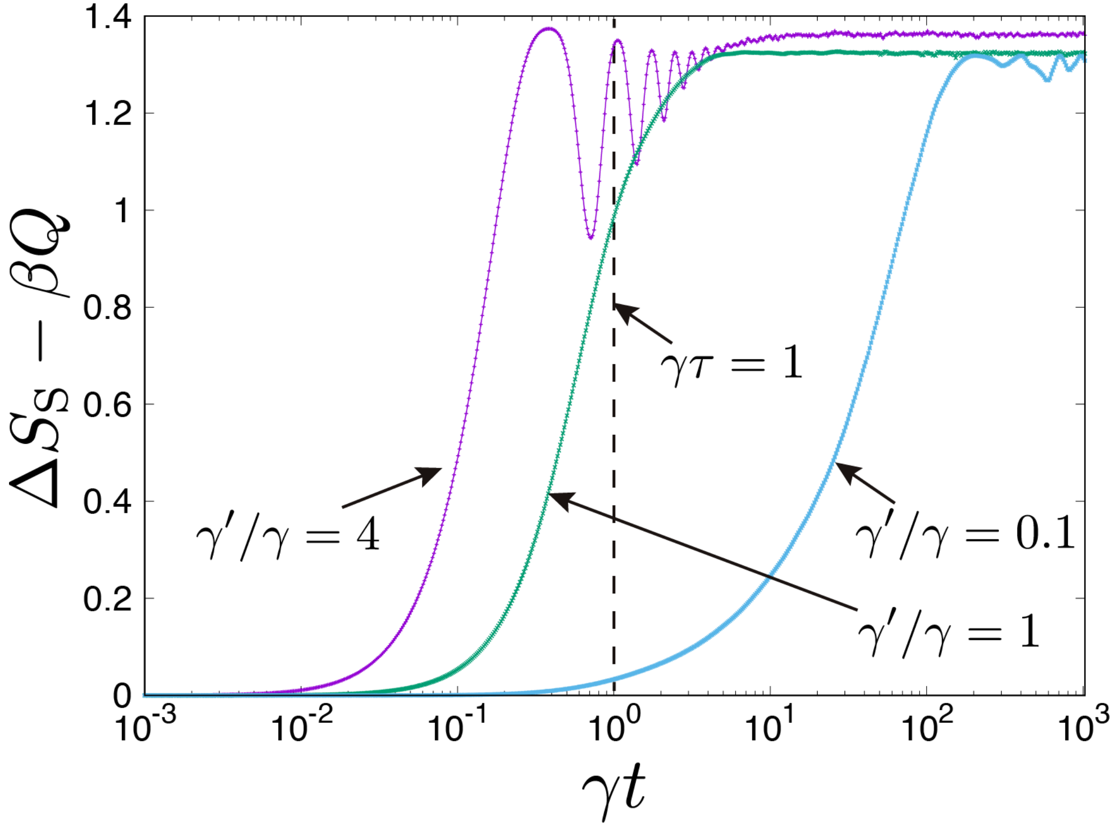
Initial state: $\hat{\rho}_{\mathrm{S}}(0) = |1\rangle\langle 1|$

Bath: 4 bosons, $\beta = 0.1$



Method: Exact diagonalization (full)

Second law



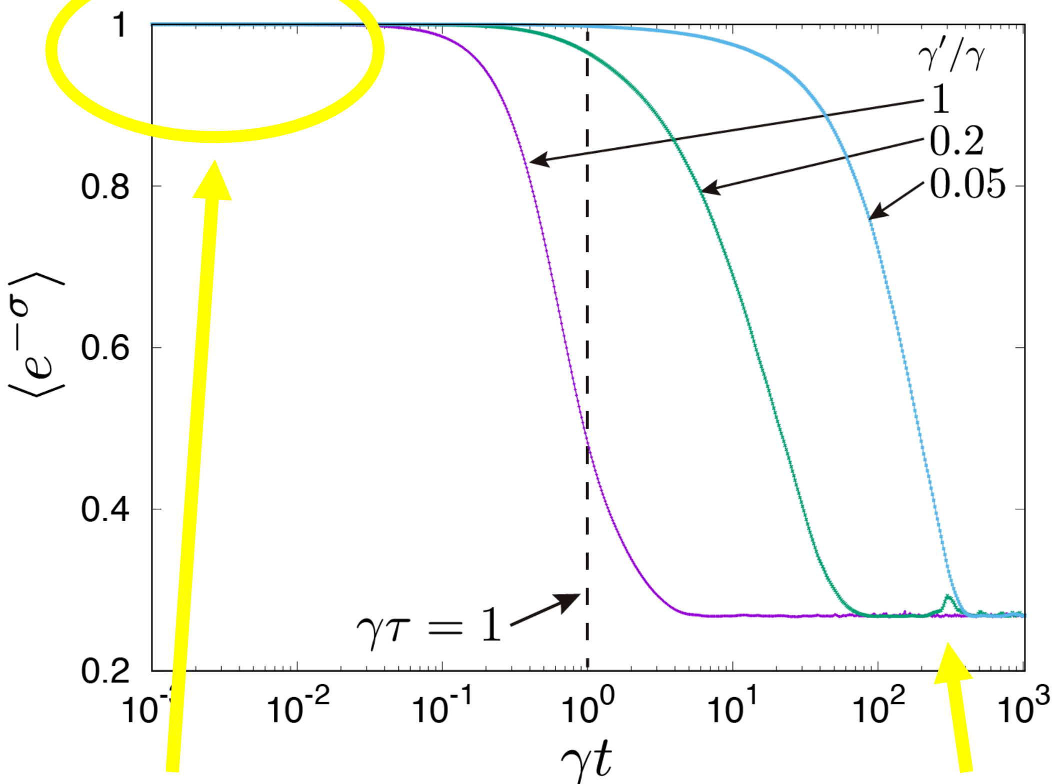
Lieb-Robinson Time $\tau \sim 1/\gamma$

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 τ

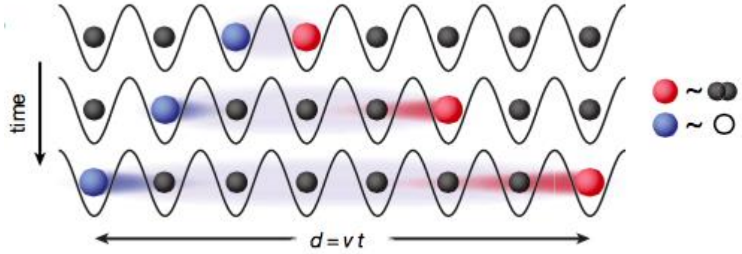
Coffee in a room: τ ~ms **very short!**

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

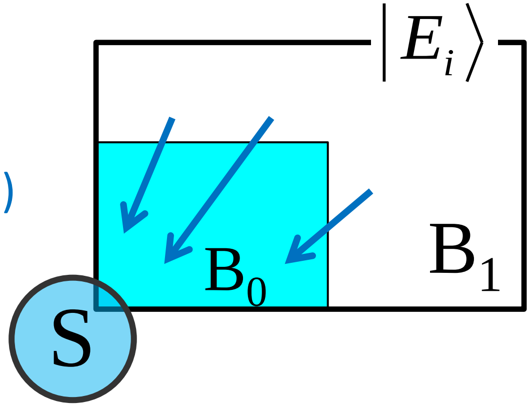


M. Cheneau *et al.*, Nature 481, 484 (2012)

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!