Universality and timescale of thermalization in isolated quantum systems

Ryusuke Hamazaki
(RIKEN CPR Hakubi, Japan)

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Refs.
*S. Sugimoto, **R. Hamazaki**, and M. Ueda, Phys. Rev. Lett. 126 (12), 120602 (2021).
*S. Sugimoto, **R. Hamazaki**, and M. Ueda, Phys. Rev. Lett. 129 (3), 030602 (2022).
***R. Hamazaki**, PRX Quantum 3 (2), 020319 (2022)

Outline

1. Introduction: thermalization of isolated quantum systems

2. Universality of thermalization in realistic systems

3. Timescale of thermalization with macroscopic transitions

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1. Introduction: thermalization of isolated quantum systems

2. Universality of thermalization in realistic systems

3. Timescale of thermalization with macroscopic transitions

How to justify equilibrium statistical mechanics from microscopic quantum dynamics?

Unitary quantum dynamics

$$\langle\psi(0)|\hat{O}|\psi(0)\rangle \longrightarrow \langle\hat{O}\rangle_{\rm mic}(E) = {\rm Tr}[\hat{O}\hat{\rho}_{\rm mic}(E)]?$$

micro-canonical ensemble

$$\hat{\rho}_{\rm mic} = \frac{1}{d_{E,\Delta E}} \sum_{|E_\alpha - E|<\Delta E} |E_\alpha\rangle\langle E_\alpha|$$

https://en.wikipedia.org/wiki/John_von_Neumann#/media/File:JohnvonNeumann-LosAlamos.gif

Fundamental problem since J. von Neumann's work (1929)

Rapid development in the current century

Experimental observation of thermalization dynamics
using artificial quantum systems, e.g., cold atoms, ions, …

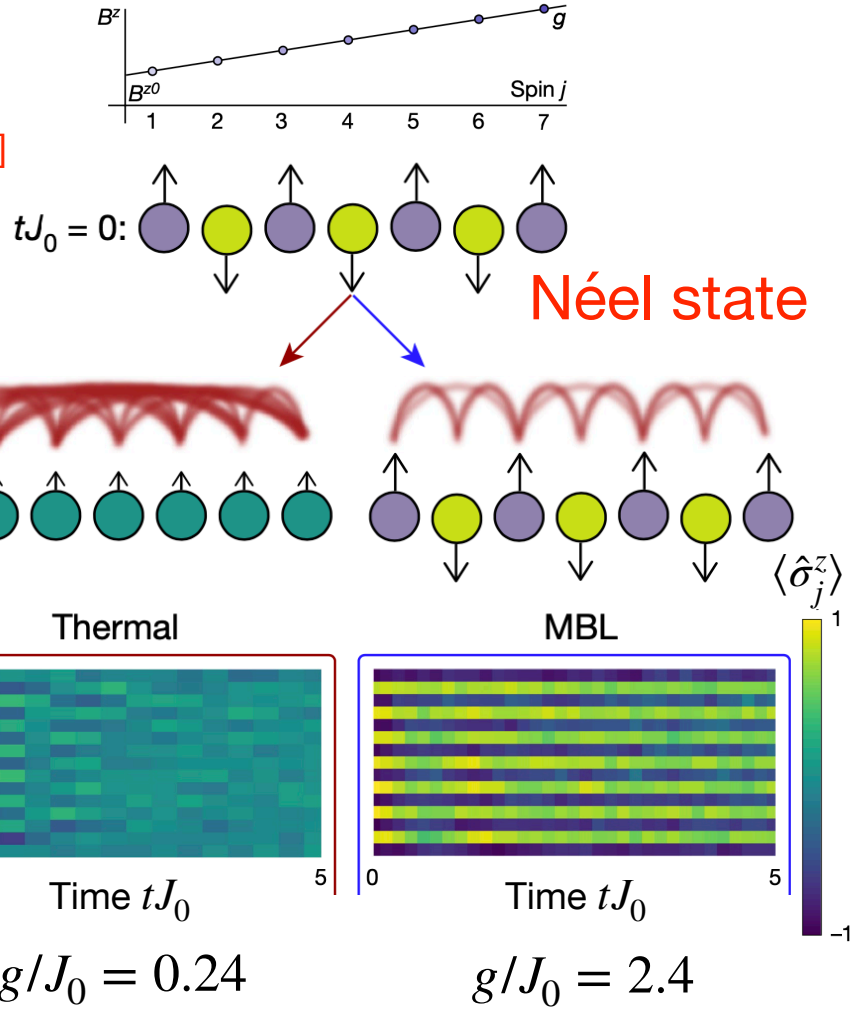
Recent experiment on thermalization and its breakdown

Trapped ions with a linear potential

[W. Morong et al., Nature 599, 393 (2021).]

$$\hat{H} = \sum_{j<j'} \frac{J_0}{|i-j|^{1.3}} \hat{\sigma}_j^x \hat{\sigma}_{j'}^x + \sum_{j=1}^{N} \left(B^{z0} + (j-1)g\right) \hat{\sigma}_{j'}^z$$

linear potential



Small g/J_0: thermalization

Large g/J_0: no thermalization
(Stark many-body localization)

$g/J_0 = 0.24$ $\quad$ $g/J_0 = 2.4$

Thermalization of isolated quantum systems is a nontrivial problem than we naively think!

Eigenstate thermalization hypothesis (ETH)

"Energy eigenstate itself behaves thermally for local observables"

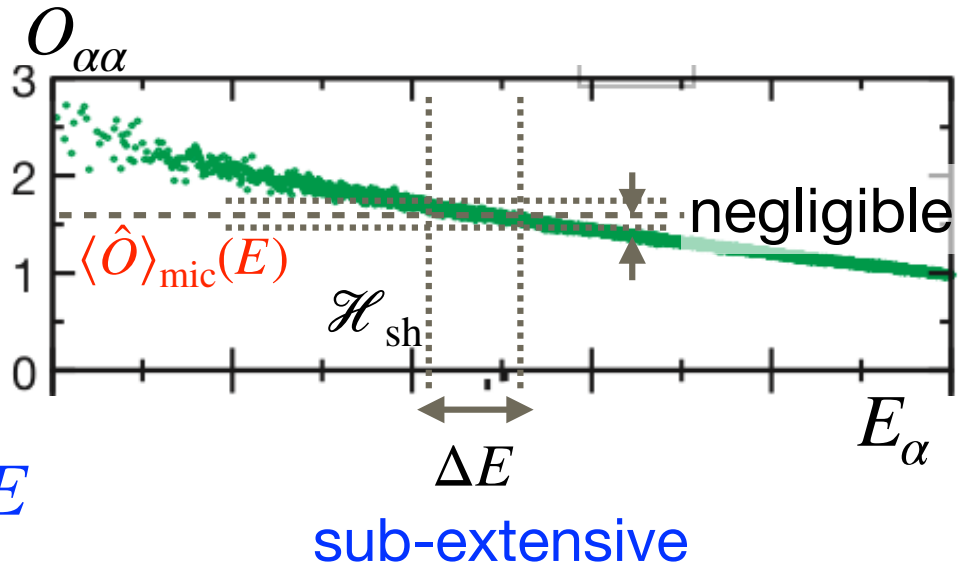
Eigenstate expectation value $O_{\alpha\alpha} = \langle E_\alpha | \hat{O} | E_\alpha \rangle$ $|E_\alpha\rangle$: energy eigenstates

ETH for $\hat{O}$:

For all $|E_\alpha\rangle \in \mathscr{H}_{\rm sh}$,

$|O_{\alpha\alpha} - \langle \hat{O} \rangle_{\rm mic}(E)|$ is negligible in the thermodynamic limit

J. von Neumann (1929); JM. Deutsch (1991); M. Srednicki (1994); M. Rigol (2008)



sub-extensive

$\mathscr{H}_{\rm sh}$: energy shell with average E and sub-extensive width ΔE

Sufficient condition for thermalization after long times for any initial state whose energy fluctuation is sub-extensive

Open questions on thermalization and the ETH

ETH has numerically been verified in many specific models

Yet, ETH-breaking systems are also found (e.g., localization)

How universal are the ETH and thermalization?

ETH ensures thermalization after infinitely long times

Yet, ETH does not tell us much about finite-time dynamics

How to evaluate timescales of thermalization?

2. Universality of thermalization in realistic systems

Collaborators: Shoki Sugimoto, Masahito Ueda (U. Tokyo)

Refs.

*S. Sugimoto, **R. Hamazaki**, and M. Ueda, Phys. Rev. Lett. 126 (12), 120602 (2021).
*S. Sugimoto, **R. Hamazaki**, and M. Ueda, Phys. Rev. Lett. 129 (3), 030602 (2022).

Von Neumann's approach to universality of thermalization

Model-independent theory to justify universality of the ETH

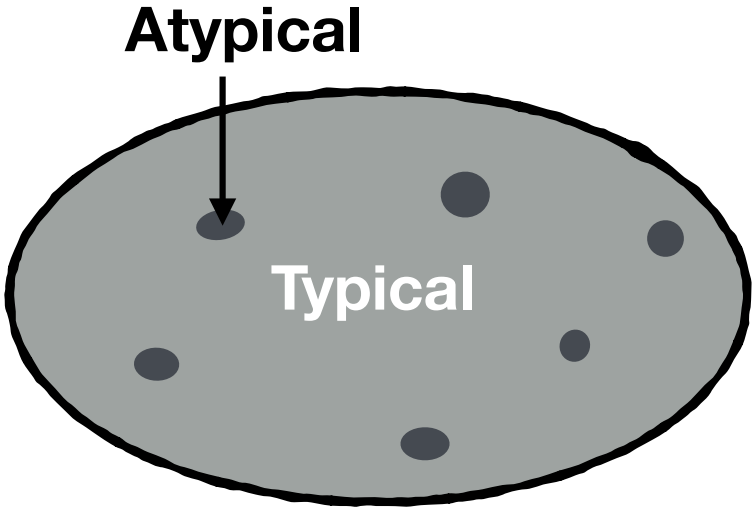
[J. von Neumann (1929); S. Goldstein et al. (2011); P. Reimann (2015).]

Consider a random Hamiltonian taken from Gaussian random matrix ensemble

$$P(H)dH \propto e^{-\mathrm{Tr}[H^2]}dH$$

→ Analytical calculation of $O_{\alpha\alpha}$

*Original paper considers the unitary Haar measure within the microcanonical energy shell



Space of all matrices

Mathematical fact: "the measure concentration"

For almost all (typical) random matrices H,
$|O_{\alpha\alpha} - \langle\hat{O}\rangle_{\mathrm{mic}}(E)|$ are exponentially small with system size

→ the ETH & thermalization

Von Neumann's approach to universality of thermalization

Model-independent theory to justify universality of the ETH

[J. von Neumann (1929); S. Goldstein et al. (2011); P. Reimann (2015).]

Atypical

Does this "typicality" indicate the universality of the ETH for *realistic* quantum many-body systems?

Von Neumann's argument conjectures so,
but we showed that this is not correct

[R. Hamazaki and M. Ueda, Phys. Rev. Lett. 120, 080603 (2018)]

For almost all (typical) random matrices H,
$|O_{\alpha\alpha} - \langle \hat{O} \rangle_{\mathrm{mic}}(E)|$ are exponentially small with system size
→ the ETH & thermalization

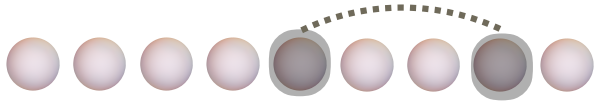
Importance of locality/few-body property

Most Gaussian random matrices contain interactions given by many-body and non-local operators

Realistic Hamiltonians are written as
a sum of few-body (and often local) operators

e.g.) $\hat{H} = \sum_j J\hat{\sigma}_j^z\hat{\sigma}_{j+1}^z$ → local, few-body (realistic)

$\hat{H} = \sum_{i,j} \frac{J}{|i-j|^\alpha}\hat{\sigma}_i^z\hat{\sigma}_j^z$ → few-body (realistic)



$\hat{H} = J\hat{\sigma}_1^z\cdots\hat{\sigma}_L^z$ → many-body (unrealistic)

Von Neumann's approach indeed fails for the setup with few-body Hamiltonians and observables

[R. Hamazaki and M. Ueda, Phys. Rev. Lett. 120, 080603 (2018)]

Universality of thermalization for physical systems

We need another approach to justify the universality of the ETH, considering few-body property

Idea:
Combining few-body property of the Hamiltonian and von Neumann's idea of using random matrix ensembles

→ Few-body random-matrix ensembles

Results:

We numerically verify the universality of the ETH/thermalization for realistic few-body Hamiltonians whose interaction range is not too long

[S. Sugimoto, **R. Hamazaki,** and M. Ueda, PRL (2021); Phys. Rev. Lett. 129 (3), 030602 (2022).]

Local random-matrix ensemble

[S. Sugimoto, **R. Hamazaki**, and M. Ueda, Phys. Rev. Lett. 126 (12), 120602 (2021).]

Consider random matrix ensemble with locality degree l

$\hat{h}^{(l)}$: local random operator
nontrivially acting on neighboring l sites

Focus on translation-invariant,
spin-1/2 one-dimensional Hamiltonians

$$\hat{H}_N = \sum_{j=0}^{N-1} \hat{T}^j \hat{h}^{(l)} \hat{T}^{-j}$$

$\hat{T}$: translation operator

Indicator of the ETH

$$\Delta_\infty = \frac{\max_\alpha |O_{\alpha\alpha} - \langle \hat{O} \rangle_{\mathrm{mic}}(E_\alpha)|}{\eta_O}$$

η_O : spectral width of $\hat{O}$

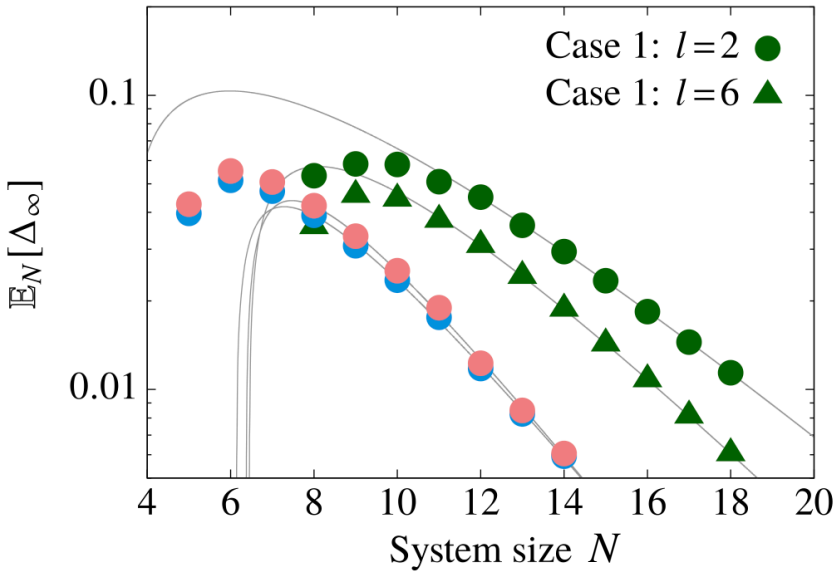
$\Delta_\infty \to 0 \ (N \to \infty)$: ETH

Numerically obtain the distribution of Δ_∞ for $\hat{H}_N$ and $\hat{O}$ taken from the local random-matrix ensemble!

Universality of the ETH

[S. Sugimoto, **R. Hamazaki**, and M. Ueda, Phys. Rev. Lett. 126 (12), 120602 (2021).]

$\mathbb{E}_N[\Delta_\infty]$: Δ_∞ over sample average



Fitting function

$$\mathbb{E}_N[\Delta_\infty] = m_0 N e^{-N/N_m}\sqrt{1-\frac{N_m}{2}\frac{\log N}{N}-\frac{N_0}{N}}$$

Markov inequality:

$$\mathrm{Prob}_N\left[\Delta_\infty \le \epsilon\right] \ge 1-\frac{\mathbb{E}_N[\Delta_\infty]}{\epsilon} \to 1-e^{-\mathrm{O}(N)} \quad (N\to\infty)$$

(Take e.g., $\epsilon \sim N^{-1}$)

→ The ETH holds for most of the local Hamiltonians!

(number of exceptions is exponentially small)

Evidence for universality of the ETH in realistic systems

Long-range random-matrix ensemble

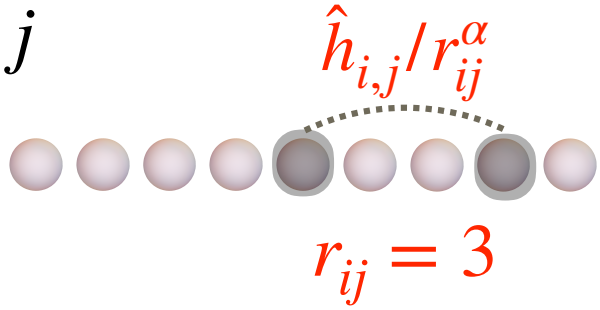
[S. Sugimoto, R. Hamazaki, and M. Ueda, Phys. Rev. Lett. 129 (3), 030602 (2022).]

Long-range interacting systems also exist (e.g., Coulomb)

Algebraically decaying interaction with tunable exponent is realized in, e.g., trapped ions B. Neyenhuis et al., Science advances 3(8), e1700672 (2017).

Universality of thermalization for long-ranged systems?

$\hat{h}_{i,j}$: random two-body operator acting on i and j



Translation invariant long-range Hamiltonians with the decay exponent α

$$\hat{H}_{N,\alpha}=\sum_{i\neq j}^{N}\frac{\hat{h}_{i,j}}{(r_{ij})^{\alpha}}$$

Calculate $\Delta_{\infty}=\dfrac{\max_{\alpha}|O_{\alpha\alpha}-\langle\hat{O}\rangle_{\mathrm{mic}}(E_{\alpha})|}{\eta_{O}}$ by changing α to see the ETH

Results

[S. Sugimoto, R. Hamazaki, and M. Ueda, Phys. Rev. Lett. 129 (3), 030602 (2022).]

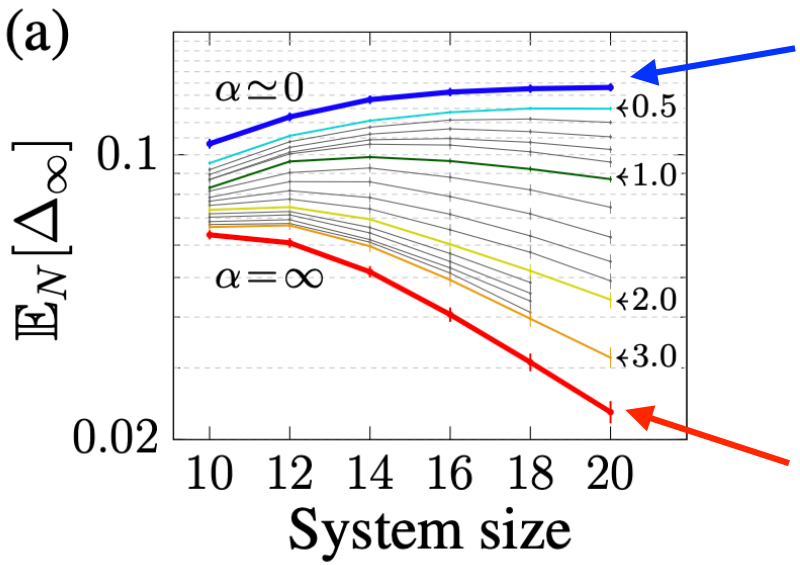
Numerics of $\mathbb{E}_N[\Delta_\infty]$ up to $N = 20$ (cf. the Markov inequality)

$\alpha \gtrsim 0.6$: **Universally of the ETH**

Probability that $\mathbb{E}_N[\Delta_\infty]$ vanishes is estimated by the bootstrap method

$\alpha \lesssim 0.5$: No evidence of the ETH (proximity to $\alpha = 0$)

Our result does not tell behaviors in the thermodynamic limit,
but is relevant for experiments with finite-size systems



Infinite range models:

having permutation symmetry for i and j

(the ETH breaks down due to
the additional conserved quantity)

Local random matrix ensemble

(ETH holds, as seen before)

3. Timescale of thermalization with macroscopic transitions

Ref.

*R. Hamazaki, PRX Quantum 3 (2), 020319 (2022)

Timescale of thermalization for isolated quantum systems

How fast can relaxation dynamics take place?

The ETH is helpless for evaluating timescales

Various approaches exist, e.g.,

*Typical relaxation relying on the Haar measure

[S. Goldstein et al, NJP (2015); P. Reimann, Nat. Commun. (2016).]

***Quantum speed limits**

Tradeoff relations between speed and physical quantities

Upper bound on instantaneous speed of an observable

$$\left| \frac{d\langle \hat{A}(t) \rangle}{dt} \right| \leq 2\Delta A(t) \cdot \Delta H$$

Total energy fluctuation limits the speed

[L. Mandelstam and I. Tamm, J. Phys. 9, 249 (1945).]

Timescale of thermalization for isolated quantum systems

How fast can relaxation dynamics take place?

The ETH is helpless for evaluating timescales

Previous approaches do not predict reasonable timescales for processes with macroscopic transitions

$$\left| \frac{d\langle \hat{A}(t) \rangle}{dt} \right| \leq 2\Delta A(t) \cdot \Delta H$$

Total energy fluctuation limits the speed

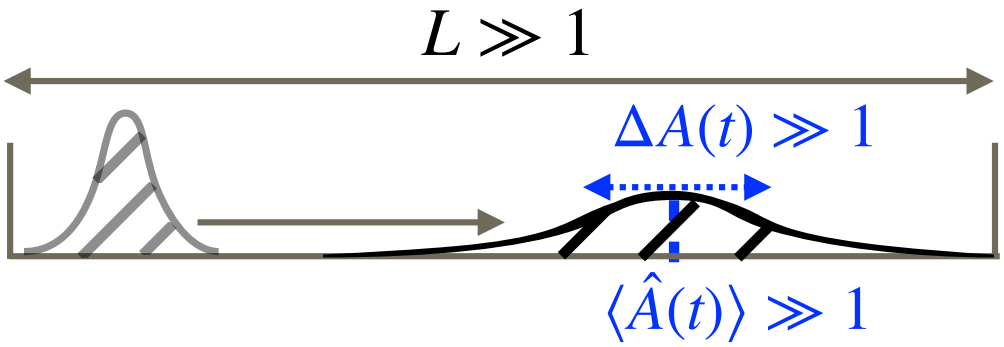
[L. Mandelstam and I. Tamm, J. Phys. 9, 249 (1945).]

Macroscopic transitions

Important relaxation process: macroscopic transport of, e.g., particles

System or displacement is much larger than the typical microscopic length-scale

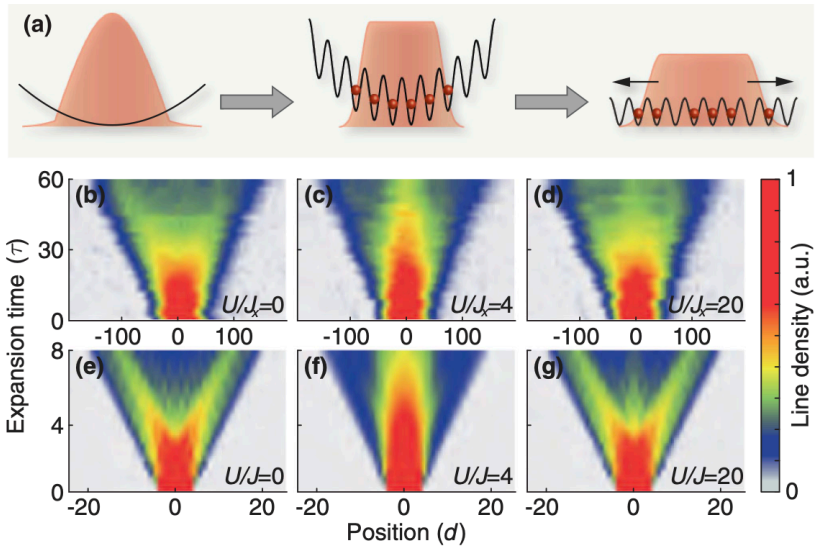
Observables of interest:
Atomic mean positions $\langle \hat{A}(t) \rangle$,
or fluctuations $\Delta A(t)$, etc…



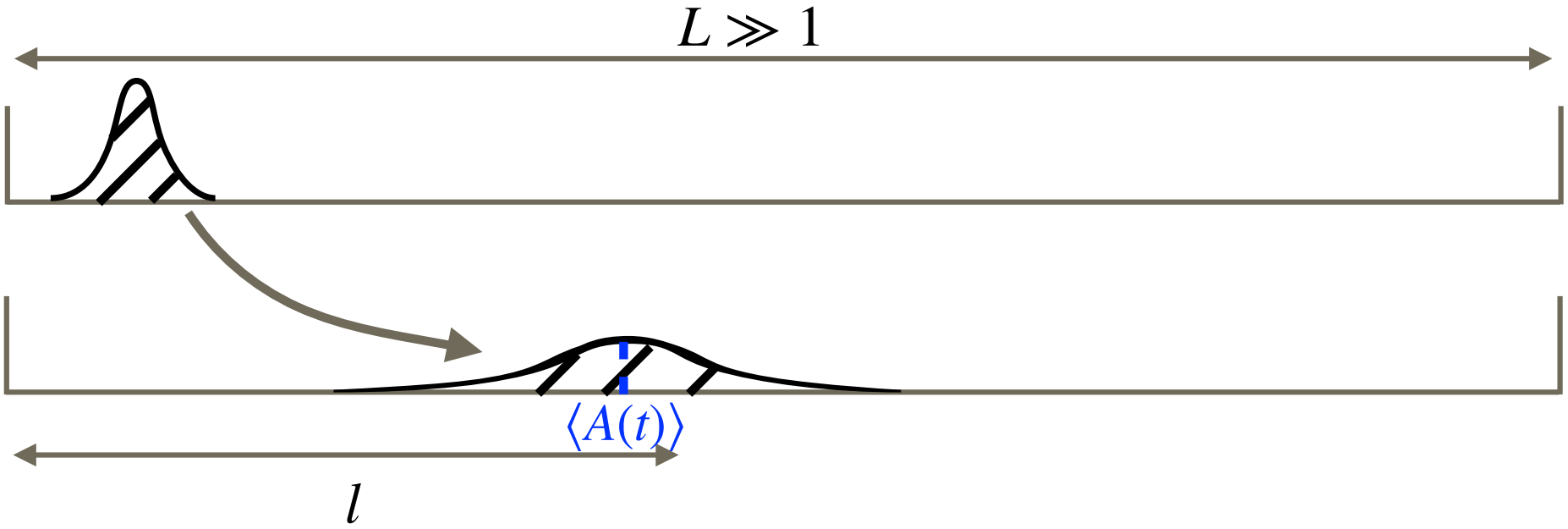
Relevant for many non-equilibrium processes, including thermalization dynamics from inhomogeneous initial states

Atomic transport experiment in cold atoms

J. P. Ronzheimer et al.,
PRL 110, 205301 (2013).



Problem for macroscopic transitions



e.g.) A: Average position of M particles

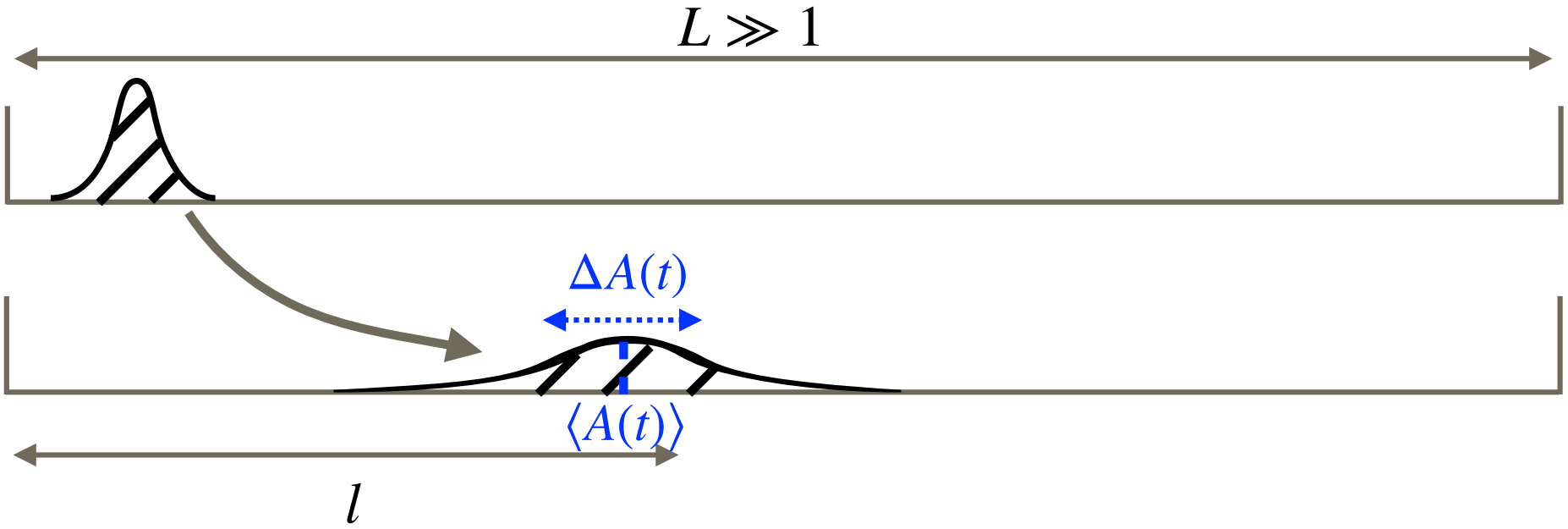
For locally interacting systems,

Instantaneous speed $\left| \frac{d\langle \hat{A}(t) \rangle}{dt} \right|$ → finite (non-increasing with L, M, t)

Relaxation time T → proportional to L or longer, $\sim \mathrm{O}(L^b)$ $(b \geq 1)$

Conventional approaches do not even predict these order!

Problem for macroscopic transitions



e.g.) A: Average position of M particles

Mandelstam-Tamm quantum speed limit

$$\left| \frac{d\langle \hat{A}(t) \rangle}{dt} \right| \leq 2\Delta A \cdot \Delta H$$

The LHS is non-increasing with L, M, t

↔ RHS typically diverges and is meaningless

$$\Delta A \sim \min(t^c, L) \quad (c > 0)$$

diverges unboundedly

We only have a loose bound on the timescale, too: $T \geq T_{\text{bound}} = \mathrm{o}(L)$

Motivation and main results

Is there a useful speed limit for macroscopic transitions?

Result

Using the local conservation law of probability,
we find speed limit based on the “gradient” of observables,
which gives the expected order of the speed/timescale

For unitary quantum systems, our bound shows that
transition part of energy E_{trans} suppresses the speed

R. Hamazaki, PRX Quantum 3 (2), 020319 (2022).

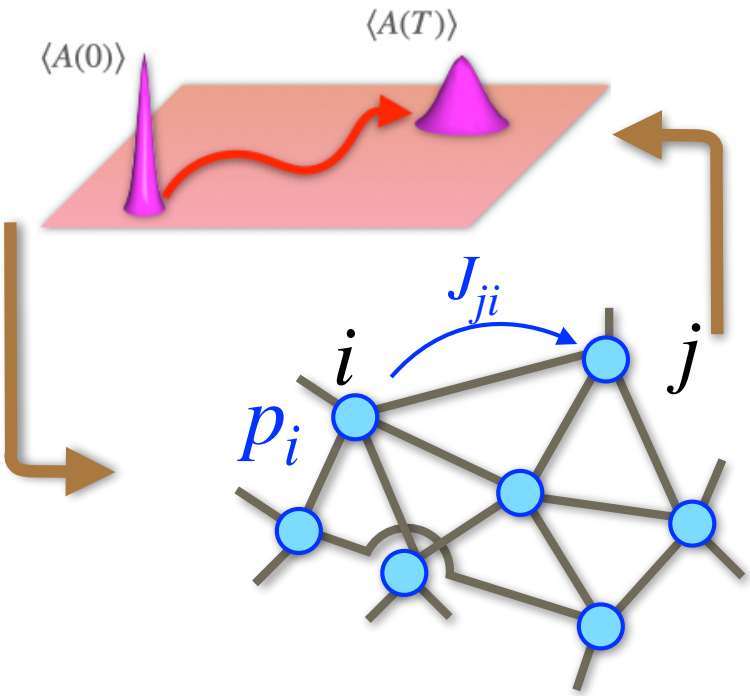
Idea

[R. Hamazaki, PRX Quantum 3 (2), 020319 (2022).]

To treat a general (discrete) system, we consider mapping it to a graph structure $G = (\mathscr{V}, \mathscr{E})$

Vertices: $i \in \mathscr{V}$ (basis of the state)

Edges: if $i \neq j$ and there is a transition between i and j, $(i, j) \in \mathscr{E}$



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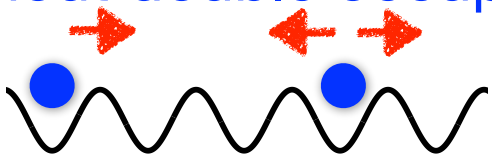
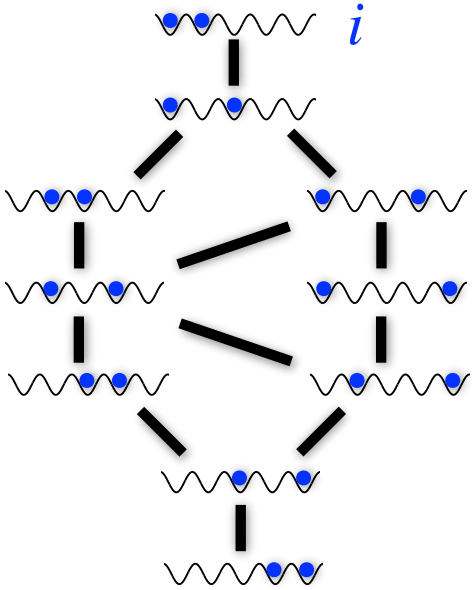
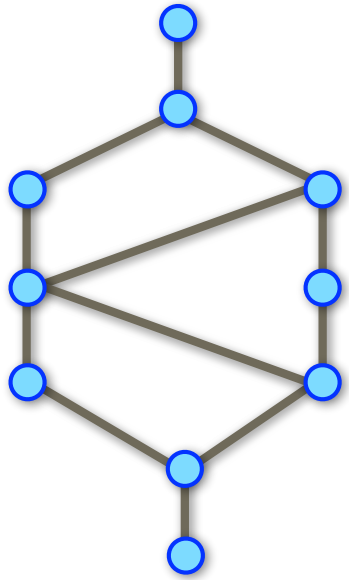
e.g.) 5 sites, 2 particles
with neighboring hopping
(without double occupancy)







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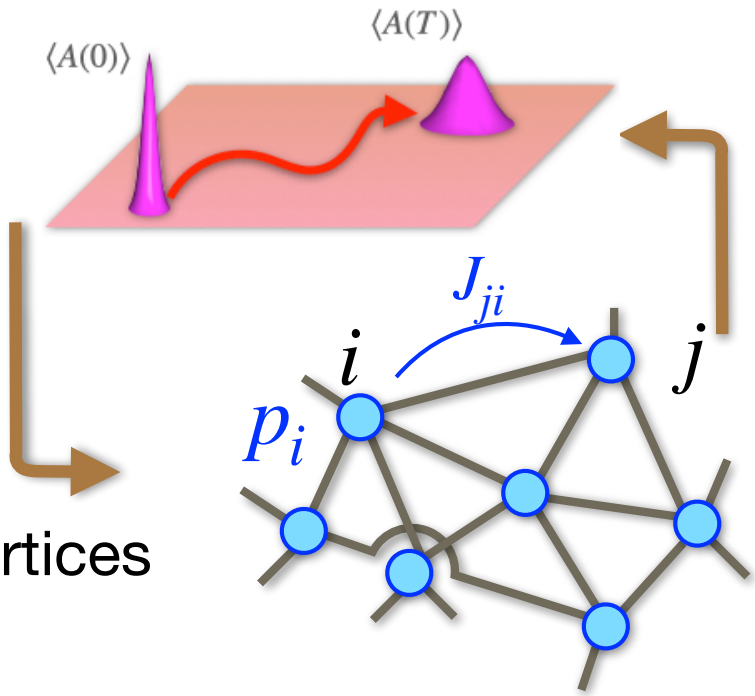


We define a probability distribution $\{p_i\}$ on vertices

For typical physical processes, we can assume the local continuity equation of probability

$$\rightarrow \quad \frac{\mathrm{d}p_i}{\mathrm{d}t} = -\sum_{j:(j,i)\in\mathscr{E}} J_{ji}(t)$$

J_{ji} : probability current from i to j

Quantum macroscopic systems

Unitary quantum dynamics $\frac{d\hat{\rho}}{dt} = -i[\hat{H}, \hat{\rho}]$ [**R. Hamazaki**, PRX Quantum 3 (2), 020319 (2022).]

Probability for the basis state $|i\rangle$: $p_i(t) = \rho_{ii}$

$$\rightarrow \frac{dp_i}{dt} = -\sum_{j:(j,i)\in\mathscr{E}} J_{ji}(t)$$

$J_{ji} = i(\rho_{ji}H_{ij} - \rho_{ij}H_{ji})$: probability current

H_{ij} : (i,j)-component of $\hat{H}$

Consider an observable with the expectation value $\langle \hat{A} \rangle = \sum_i A_i p_i(t)$

After some calculations, we obtain

$$\left| \frac{d\langle \hat{A}(t) \rangle}{dt} \right| \leq \|\nabla A\|_\infty \sqrt{C_H^2 - E_{\text{trans}}^2}$$

Quantum macroscopic systems

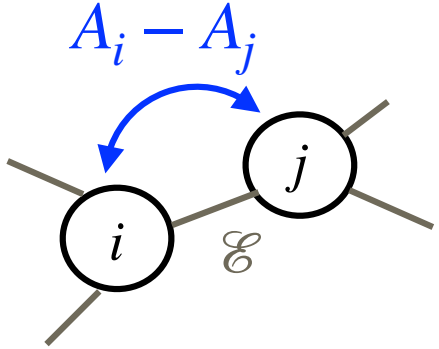
[R. Hamazaki, PRX Quantum 3 (2), 020319 (2022).]

$$\left| \frac{d\langle \hat{A}(t) \rangle}{dt} \right| \leq \|\nabla A\|_\infty \sqrt{C_H^2 - E_{\rm trans}^2}$$

$$E_{\rm trans} = \left\langle \sum_{(i,j)\in\mathscr{E}} H_{ij} \right\rangle$$ Transition energy (macroscopic observable)

$$C_H := \max_{i\in\mathscr{V}} \sum_{j:(j,i)\in\mathscr{E}} |H_{ij}|$$ Strength of transition (easily known from H)

$$\|\nabla A\|_\infty := \max_{(i,j)\in\mathscr{E}} |A_i - A_j|$$ Magnitude of "gradient" of A defined by the edges $\mathscr{E}$



***Transition energy $E_{\rm trans}$ suppresses the bound**

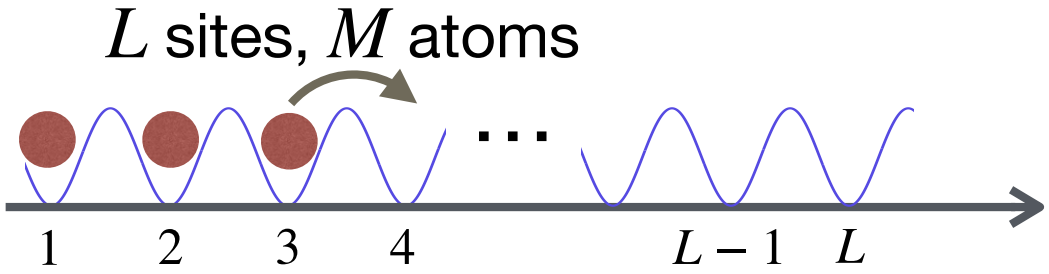
***Useful speed limits:**

$\|\nabla A\|_\infty$ does not diverge even for macroscopic transitions, unlike ΔA

Example

$$\left|\frac{d\langle\hat{A}(t)\rangle}{dt}\right| \leq \|\nabla A\|_\infty \sqrt{C_H^2 - E_{\text{trans}}^2}$$

[**R. Hamazaki**, PRX Quantum 3 (2), 020319 (2022).]



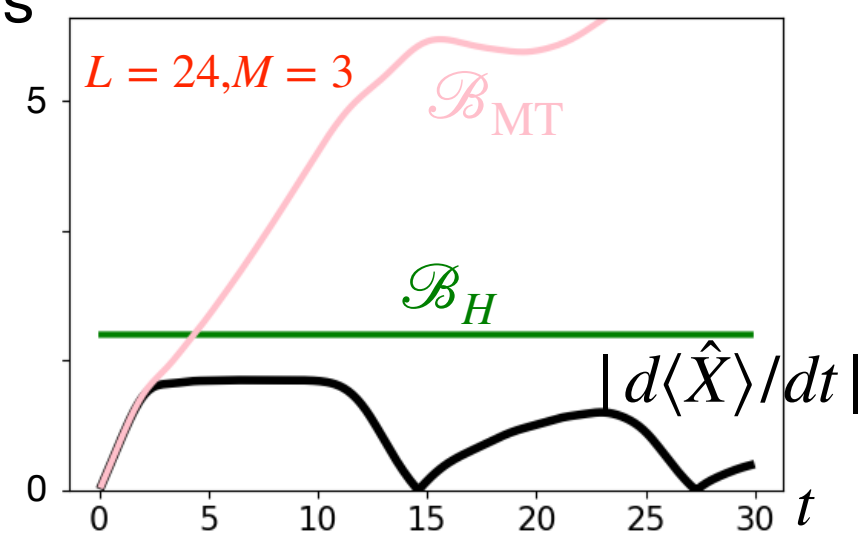
e.g.) Mean position $\hat{X}$ for interacting systems with M fermions (hopping rate K)

Our bound: finite

$$\left|\frac{d\langle\hat{X}(t)\rangle}{dt}\right| \leq \mathscr{B}_H = \sqrt{(2K)^2 - (E_{\text{trans}}/M)^2}$$

$$\ll \mathscr{B}_{\text{MT}} = 2\Delta X \Delta H$$

Mandelstam-Tamm bound: divergent



We also have tightened lower bound of the thermalization time on $\hat{X}$:

$$T \geq \frac{\mathrm{O}(L)}{\sqrt{(2K)^2 - (E_{\text{trans}}/M)^2}}$$

$$\overline{Z} = \frac{1}{T}\int_0^T dt Z(t)$$

proportional to L, as desired (unlike previous approaches)

Summary

Universality and timescale of thermalization in isolated quantum systems

Numerical verification of the universality of the ETH in realistic systems whose interaction range is not too long

*S. Sugimoto, **R. Hamazaki**, and M. Ueda, Phys. Rev. Lett. 126 (12), 120602 (2021).
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Quantum speed limits useful for macroscopic transitions based on local conservation law of probability

*__R. Hamazaki__, PRX Quantum 3 (2), 020319 (2022)