The problem of thermalization in isolated quantum many-body systems

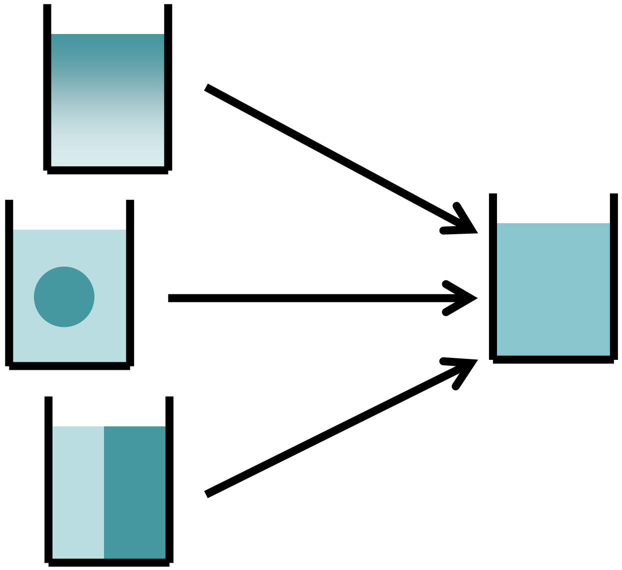
Naoto Shiraishi (University of Tokyo)

N. Shiraishi and T. Mori, Phys. Rev. Lett. 119, 030601 (2017)
T. Mori and N. Shiraishi, Phys. Rev. E 96, 022153 (2017)
N. Shiraishi, J. Stat. Mech. 083103 (2019)
N. Shiraishi and K. Matsumoto, Nat. Comm. 12, 5084 (2021)

Thermalization of macroscopic system

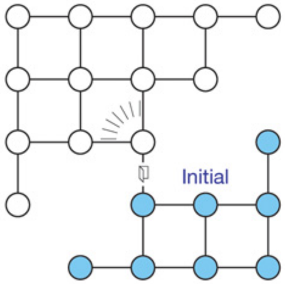
Thermalization

Non-equilibrium state goes to a unique equilibrium state (i.e., macroscopically indistinguishable).

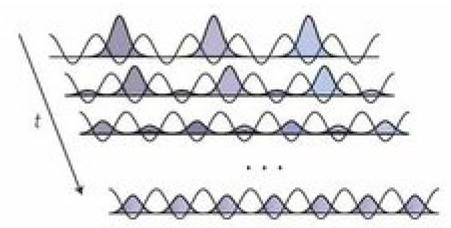


It is true for a macro **pure quantum state**.

Numerical simulation



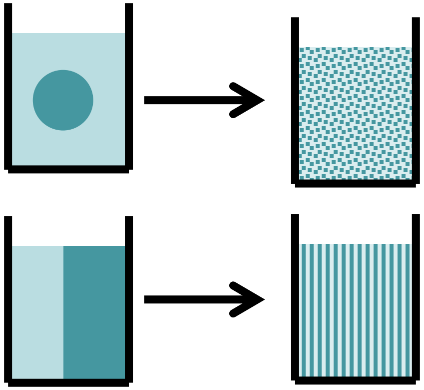
Experiment



(M. Rigol, V. Dunjko & M. Olshanii, Nature **452**, 854 (2008), M. Gring, et.al., Science 348, 207 (2015))

Why some systems thermalize while some others do not?

Some systems **do not thermalize!** (relax to initial-state-dependent ensemble)



Ex) Integrable system
- Free Fermion system
- Bethe anzats

Localized system
- Anderson localization
- Many body localization

Many researchers investigate **what determines presence/absence of thermalization**.

Outline

Part 1: General framework to violate ETH

- Background
- Construction of Hamiltonian
- Dynamics

Part 2: Undecidability of thermalization

- Main claim
- Construction of classical TM
- Quantum emulation

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Candidate: Eigenstate thermalization hypothesis

Thermal (w.r.t A)

State $|\psi\rangle$ is thermal w.r.t. A if $\langle\psi|A|\psi\rangle \simeq \mathrm{Tr}[A\rho_{\mathrm{MC}}]$

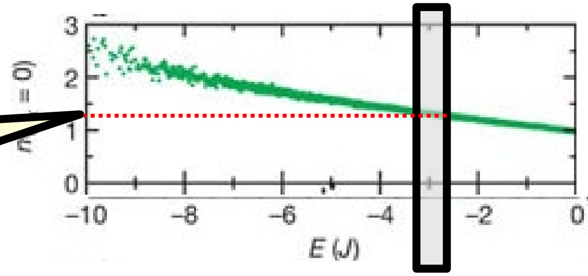
Eigenstate thermalization hypothesis (ETH)

All energy eigenstates are thermal

$\boldsymbol{\langle E_n|A|E_n\rangle \simeq \mathrm{Tr}[A\rho_{MC}]}$ (A: macro observable)

(J. von Neuman, Z. Phys. 57, 30 (1929), J. M. Deutsch, PRA 43, 2046 (1991), M. Srednicki, PRE 50, 888 (1994))

Observable takes the same value (=equilibrium value)



Plot of $\langle E_n|A|E_n\rangle/L$ versus E_n

Known properties of ETH

- **ETH is sufficient for thermalization.**
- **Many complex (non-integrable, non-localized) systems satisfy ETH.**

  L. F. Santos and M. Rigol, Phys. Rev. E 81, 036206 (2010).
  R. Steinigeweg, J. Herbrych, and P. Prelovsek, Phys. Rev. E 87, 012118 (2013).
  H. Kim, T. N. Ikeda, and D. A. Huse, Phys. Rev. E 90, 052105 (2014).
  W. Beugeling, R. Moessner, and M. Haque, Phys. Rev. E 89, 042112 (2014).
  T. Yoshizawa, E. Iyoda, and T. Sagawa, Phys. Rev. Lett. 120, 200604 (2018).

- **All known counterexamples to ETH are only non-thermalizing systems.**

  - Integrable systems (with local conserved quantities)
  - Localized systems

Beliefs on ETH

Belief

(1) ETH is satisfie … lex systems such that

- non-integra … e (no … onserved quantity)
- shift-invariant (which … ies no localization)
- local interaction

(2) ETH is necessary … hermalization.

complex systems ⇨ ETH ⇨ thermalization

… TH ⇨ no thermalization

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Example: S=1 spin chain

Consider **spin-1 chain** with p.b.c. with length L.

Projection operator: $P_i^z = \begin{cases} 0: & S_i^z = \pm 1 \\ 1: & S_i^z = 0 \end{cases}$

$$\boldsymbol{H_{\mathrm{trial}} = \sum_i P_i^z h_i P_i^z}$$

h_i: Arbitrary local Hamiltonian.

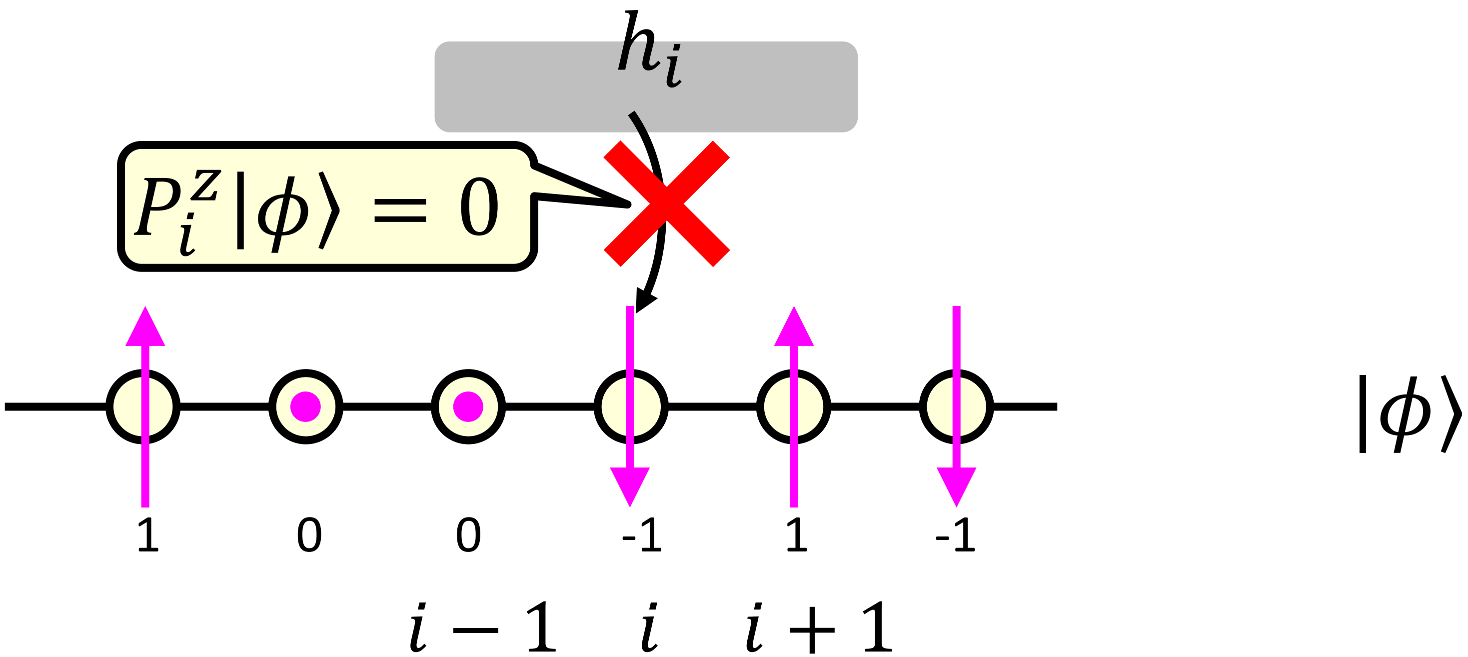
Ex) $h_i = S_{i-1}^+ S_{i+1}^- + S_{i-1}^- S_{i+1}^+$

(NS and T. Mori, Phys. Rev. Lett. 119, 030601 (2017))

Role of projection operators

$$H_{\text{trial}} = \sum_i P_i^z h_i P_i^z$$

Let us consider the case that H_{trial} acts on $|\phi\rangle$.



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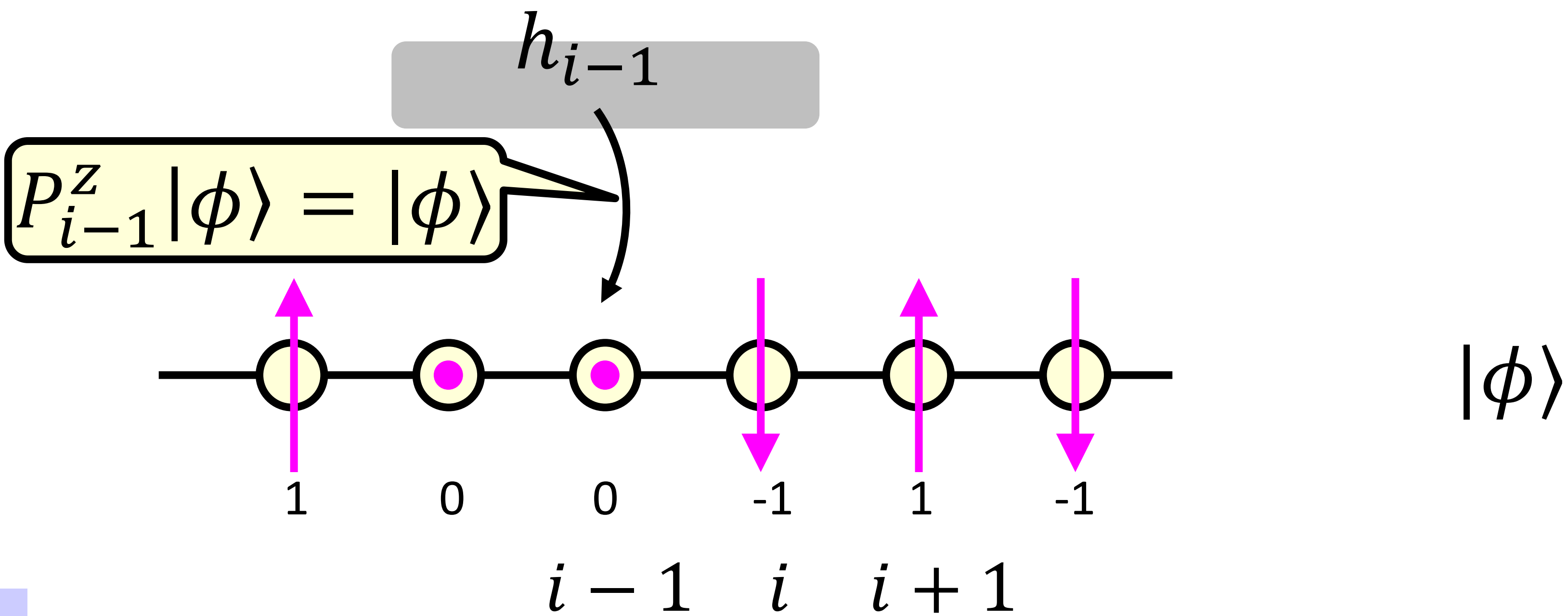
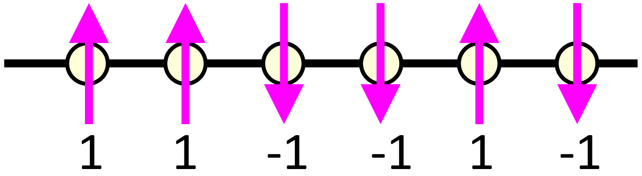
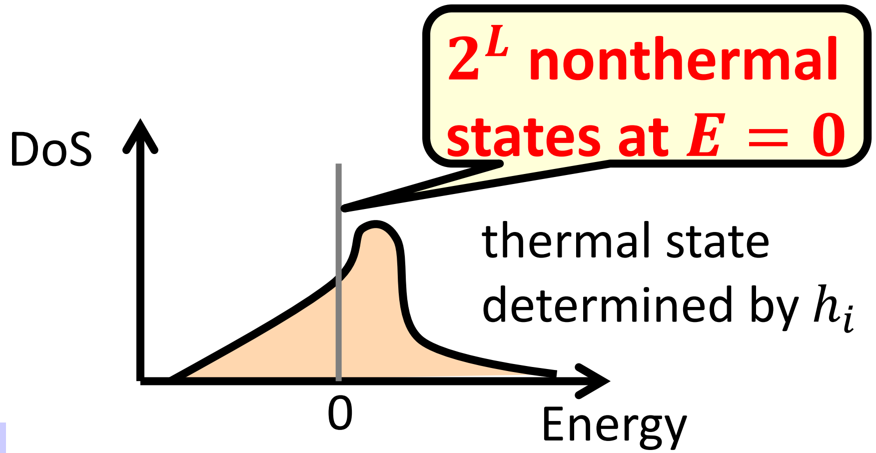


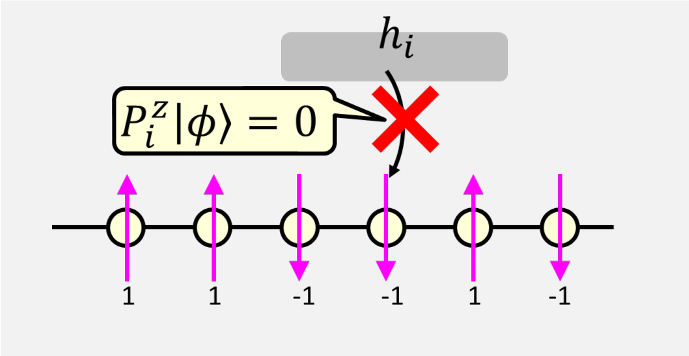
2^L eigenstates with zero energy

$\mathcal{T}$: 2^L states with all spins at ± 1



They are eigenstates of H_{trial} with zero energy!
($\because$ $|\psi\rangle \in \mathcal{T}$ satisfies $\boldsymbol{P_i^z|\psi\rangle = 0}$ for all i).



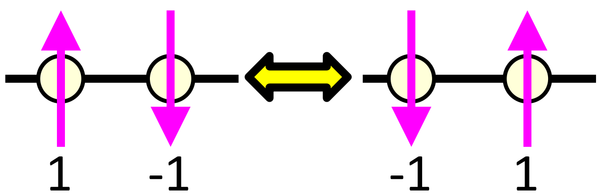


Resolving 2^L degeneracy

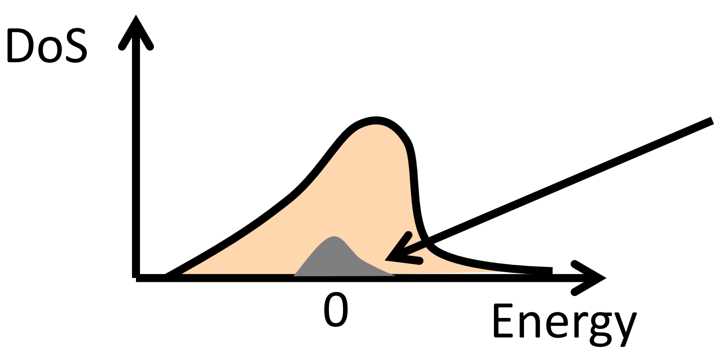
$$\boldsymbol{H} = \sum_{\boldsymbol{i}} \boldsymbol{P_i^z h_i P_i^z} + \boldsymbol{H'}$$

H': Arbitrary Hamiltonian acting only on $|1\rangle$ and $|-1\rangle$

Ex)



If $|\psi\rangle \in \mathcal{T}$, then $H'|\psi\rangle \in \mathcal{T}$.



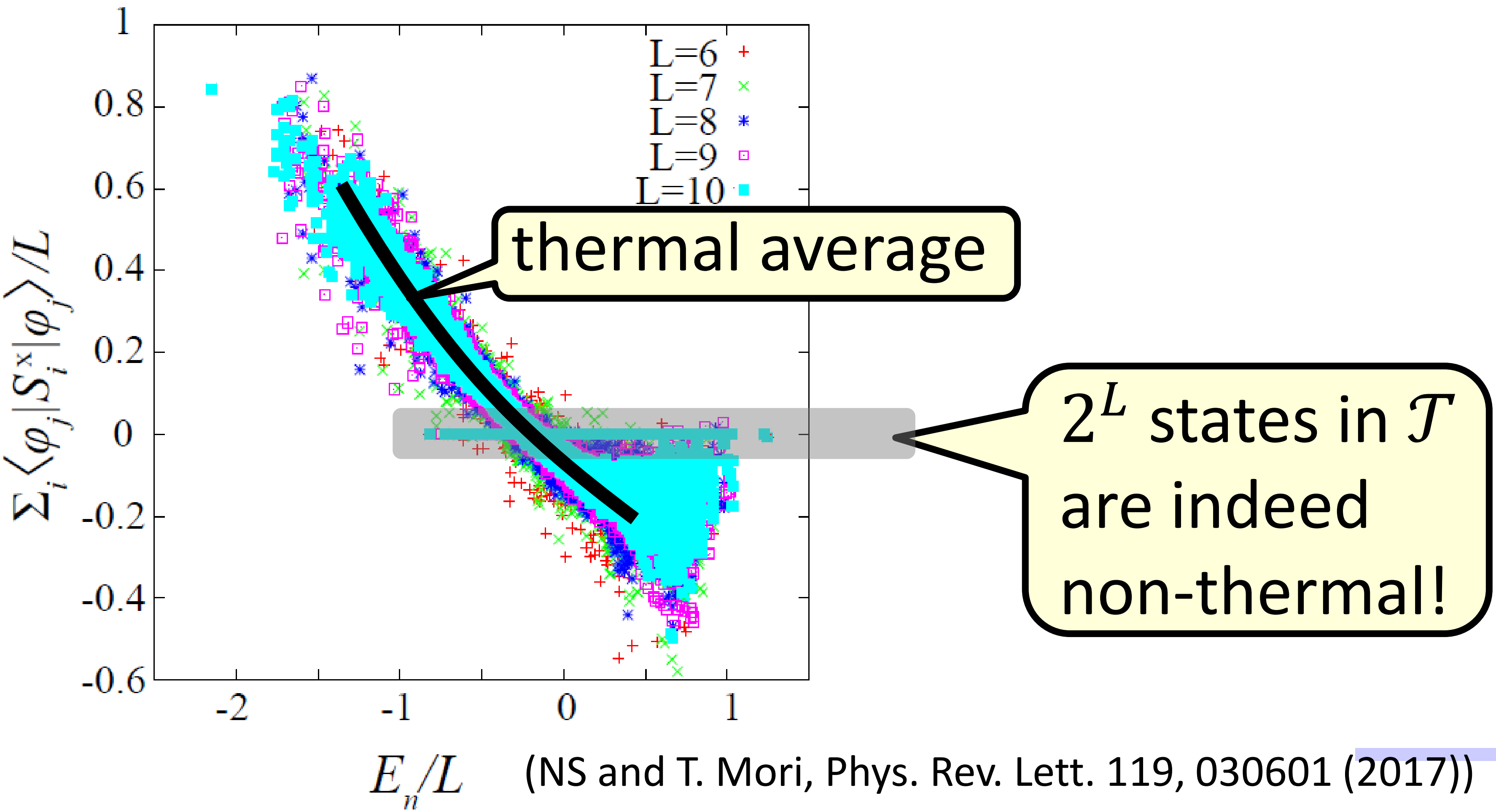
States in $\mathcal{T}$ are still non-thermal eigenstates (independent of h_i).

→**Violation of ETH!**

(NS and T. Mori, Phys. Rev. Lett. 119, 030601 (2017))

Confirming violation of ETH

Plot of $\langle E_n|\hat{O}|E_n\rangle/L$ versus E_n/L



(NS and T. Mori, Phys. Rev. Lett. 119, 030601 (2017))

Generalization: Method of embedding

$\mathcal{T}$: **target states** we want to embed

P_i: local projection operators

$$|\psi\rangle \in \mathcal{T} \Rightarrow P_i|\psi\rangle = 0$$

Then, the Hamiltonian with arbitrary h_i

$$\boldsymbol{H = \sum_i P_i h_i P_i + H'}$$

has the **target states** $\mathcal{T}$ as its **eigenstates**.

(H': satisfying $[H', P_i] = 0$ for all i)

Any **MPS** (matrix-product state) can be target state!

(ex: AKLT, dimer states, Schrodinger's cat...)

(NS and T. Mori, Phys. Rev. Lett. 119, 030601 (2017))

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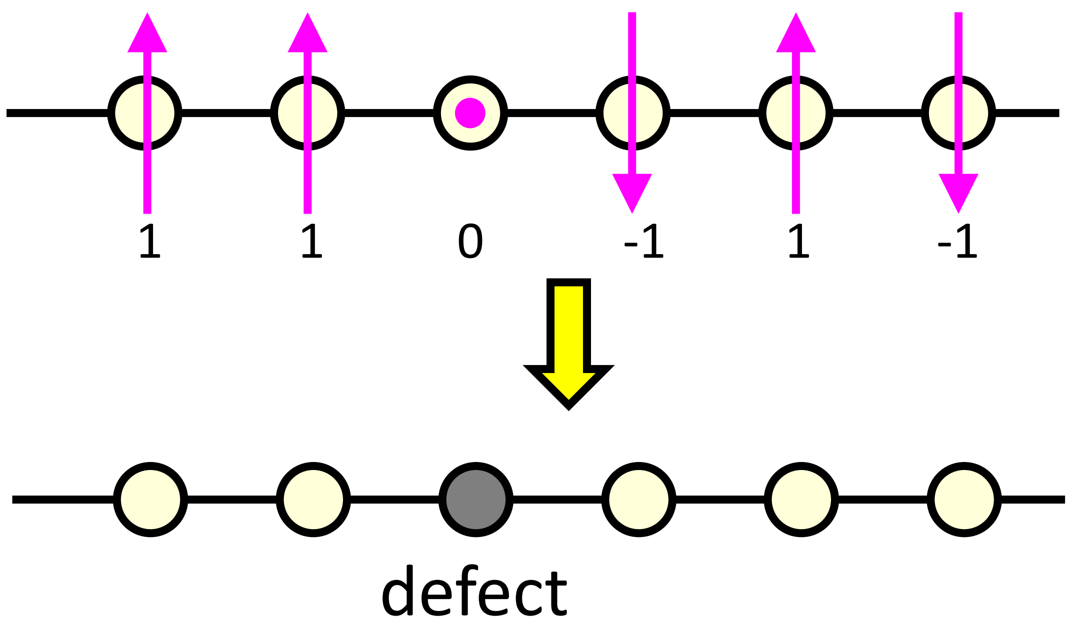
What type of initial state thermalizes?

States with all spins ± 1 never thermalize.

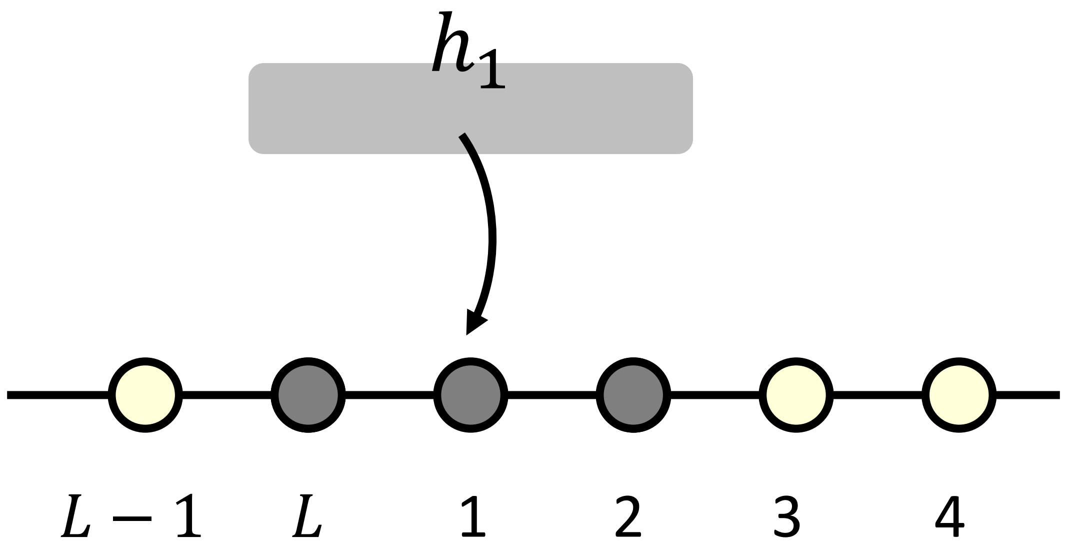
What about a state with a single spin 0?

Single spin 0 is sufficient for thermalization!

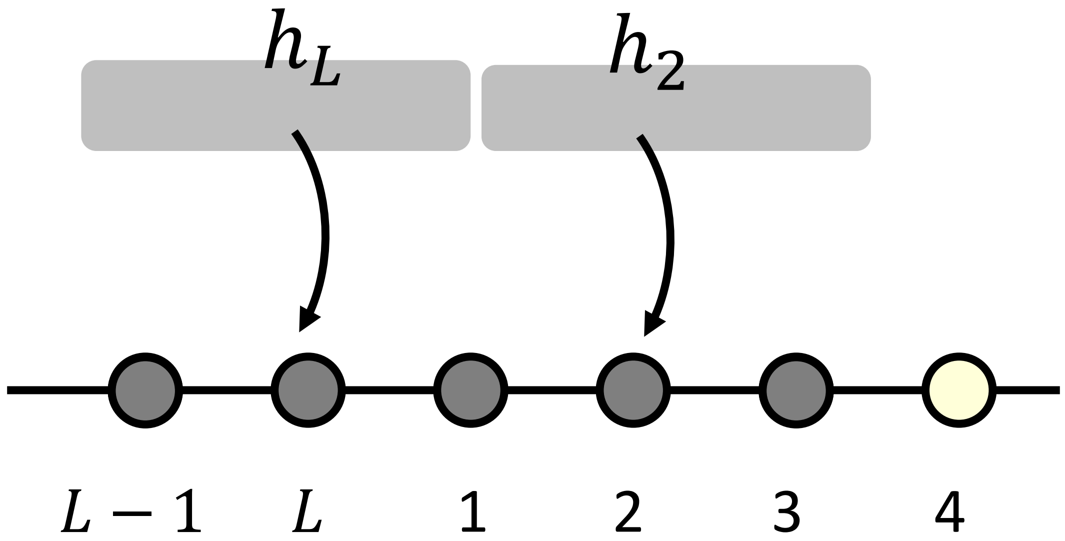


(T. Mori and NS, Phys. Rev. E 96, 022153 (2017))

Thermalization: schematic picture



Thermalization: schematic picture



Defects can spread among whole system!

Quench in macroscopic systems

Is initial state with zero defect preparable?

Quench from ground state ($T = 0$) → **Yes**

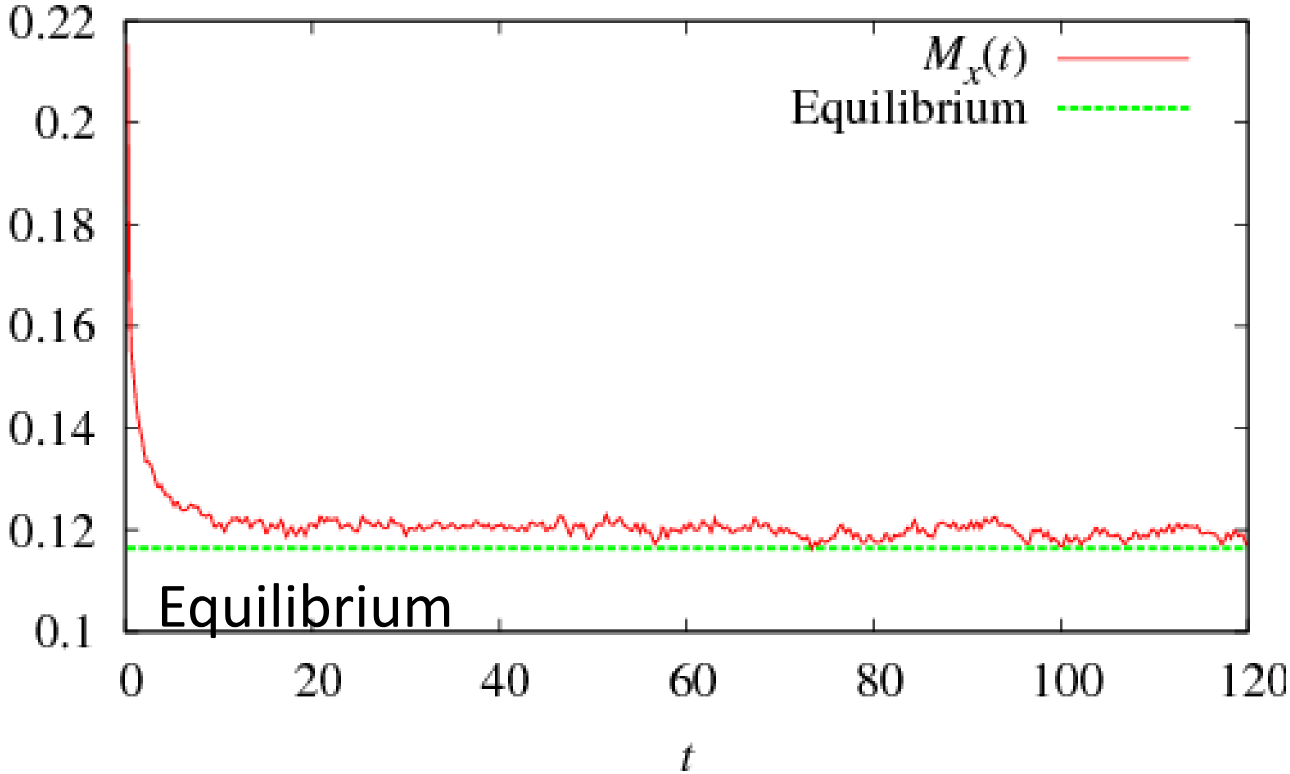
Quench from thermal state ($T > 0$) → **No!**
(Zero-defect state realizes with very small prob.)

Absolute zero temperature is unreachable.
→**physical quench inevitably contain defects**.

(T. Mori and NS, Phys. Rev. E 96, 022153 (2017))

Thermalization without ETH

Quench from thermal state of different Hamiltonian.

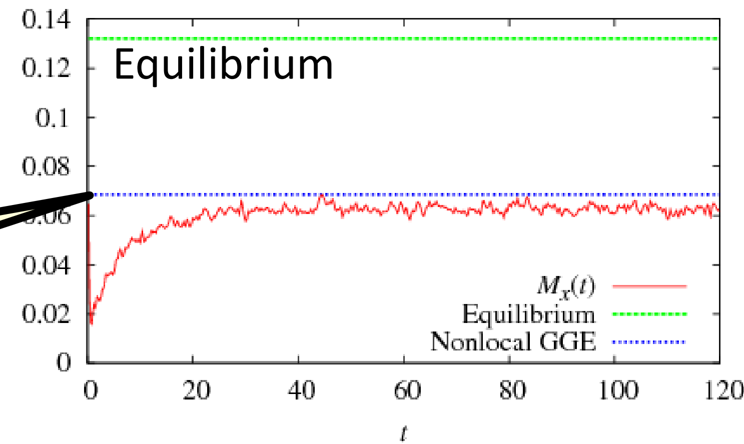


Thermalization indeed occurs!

(T. Mori and NS, Phys. Rev. E 96, 022153 (2017))

Non-local conserved quantity matters to macroscopic physics

Small system, low temperature
→thermalization may disappear!



Stationary state: **nonlocal GGE** (generalized Gibbs ensemble)

$$\rho_{GGE} \propto e^{-\beta_P \mathcal{P}H\mathcal{P} - \beta_Q \mathcal{Q}H\mathcal{Q} - \lambda \mathcal{Q}}$$

$\mathcal{Q} \coloneqq \prod_i (1 - P_i)$:**nonlocal** projection operator to $\mathcal{T}$

$\mathcal{P} \coloneqq 1 - \mathcal{Q}$

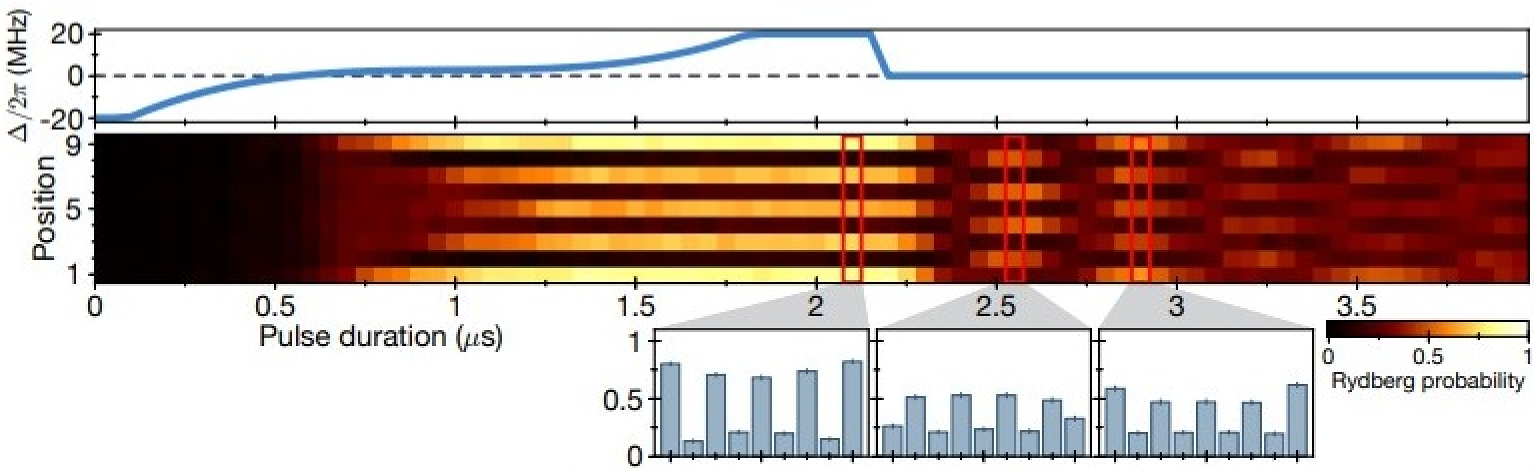
$\beta_P, \beta_Q, \lambda$: depend on initial state

(T. Mori and NS, Phys. Rev. E 96, 022153 (2017))

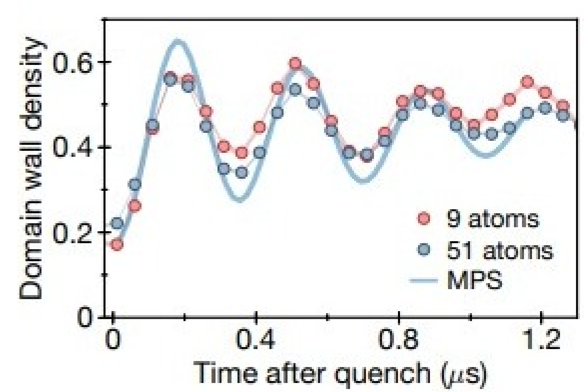
Quantum many-body scars

Experiment of Rydberg atoms

(H. Bernien, et al. Nature 551, 579 (2017))



Initial-state-dependent long-lived oscillation (Quantum many-body scar) is observed.



Quantum many-body scar is a kind of embedded Hamiltonian

PXP model (effective Hamiltonian of scar system) is nonintegrable, but some eigenstates are nonthermal, which can be explicitly solvable.

(C.-J. Lin and O. I. Motrunich, Phys. Rev. Lett. 122, 173401 (2019)).

(Mapped) PXP model is written as an **embedded Hamiltonian** which embeds **AKLT state**.

(NS, J. Stat. Mech. 083103 (2019)).

In fact, most of models of quantum many-body scars are also embedded Hamiltonians.

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Question

ETH is not a general answer for thermalization.

What determines the presence/absence of thermalization?

To investigate this question, we employ a simple setup: 1d spin chain with d local states.

Statement of decision problem

Arbitrarily given parameters

Observable：spatial average of 1-body observable

$$\boldsymbol{A} = \frac{\boldsymbol{1}}{\boldsymbol{L}} \sum_{\boldsymbol{i}} \boldsymbol{a}_{\boldsymbol{i}} \text{ (}a\text{ is arbitrary)}$$

Initial state：$|\phi_0\rangle \otimes |\phi_1\rangle \otimes |\phi_1\rangle \otimes \cdots \otimes |\phi_1\rangle$

($\langle\phi_0|\phi_1\rangle = 0$)

Input：-$d^2 \times d^2$ local Hamiltonian h

System Hamiltonian is $\boldsymbol{H} = \sum_{\boldsymbol{i}} \boldsymbol{h}_{\boldsymbol{i},\boldsymbol{i}+\boldsymbol{1}}$

-Target value A^* (In case of undecidability of relaxation.)

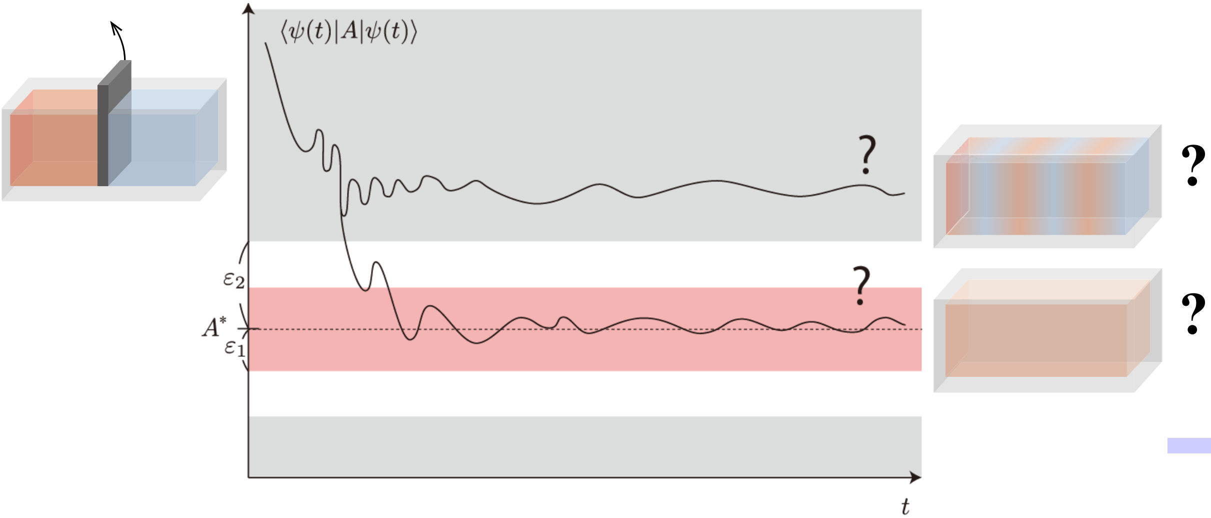
Statement of decision problem

<u>Decision problem with promise</u>

Decide whether the difference between

- $\bar{A}$ (long time average of A: determined by $H, |\psi\rangle, A$)
- a given value A^*

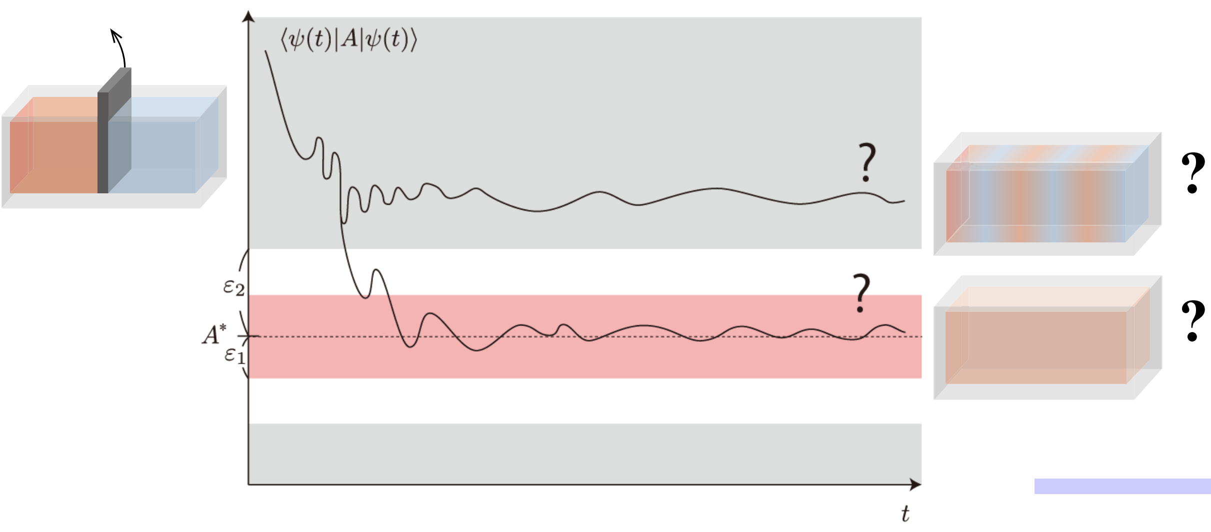
is (1) less than ϵ_1, or (2) larger than ϵ_2 ($> \epsilon_1$) in the thermodynamic limit.



Main result: undecidability of thermalization

<u>Theorem</u>：Given $A, |\psi(0)\rangle$ and fix. The presence or absence of thermalization is **undecidable**. (For given H, no procedure determines the presence/absence of thermalization.) (NS and K. Matsumoto, Nat. Comm. 12, 5084 (2021))

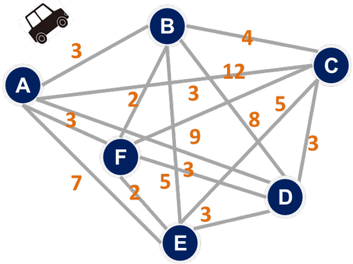
It is easy to set A^* to the equilibrium value A_{eq}, which is undecidability of thermalization.



Decidable/undecidable

<u>Decidable</u>：There exists a procedure (algorithm) which answers Yes/No correctly for any input.
(Remark: it can take extremely long time)

Ex)
- Proven in the form of theorem
- Optimization (ex: traveling salesman problem)



- Whether black/white wins in (generalized) Go.

- Indefinite integration $\int dx \frac{e^{\sin x}}{x^2 + \cos x} = ?$
- First order real closed field (problem with four arithmetic operation and inequality in real number)

Decidable/undecidable

Decidable：There exists a procedure (algorithm) which answers Yes/No correctly for any input. (Remark: it can take extremely long time)

Undecidable：There is no procedure/algorithm which decides Yes/No correctly (Of course, there is no general theorem)

(Related to Godel's incompleteness theorem)

Undecidability of halting problem

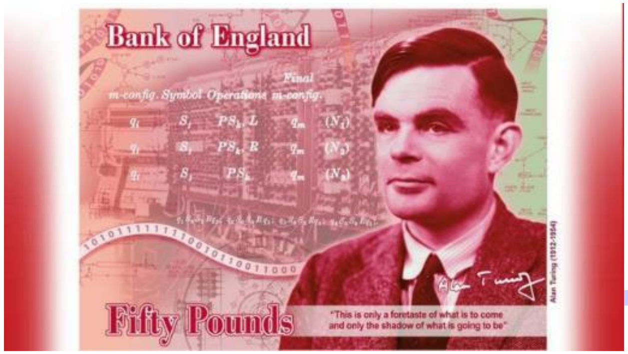
Halting problem of Turing machine (TM)

Input: an input for a given universal TM.

Problem: Does universal TM with this input "halt at some time" or "not halt forever"?

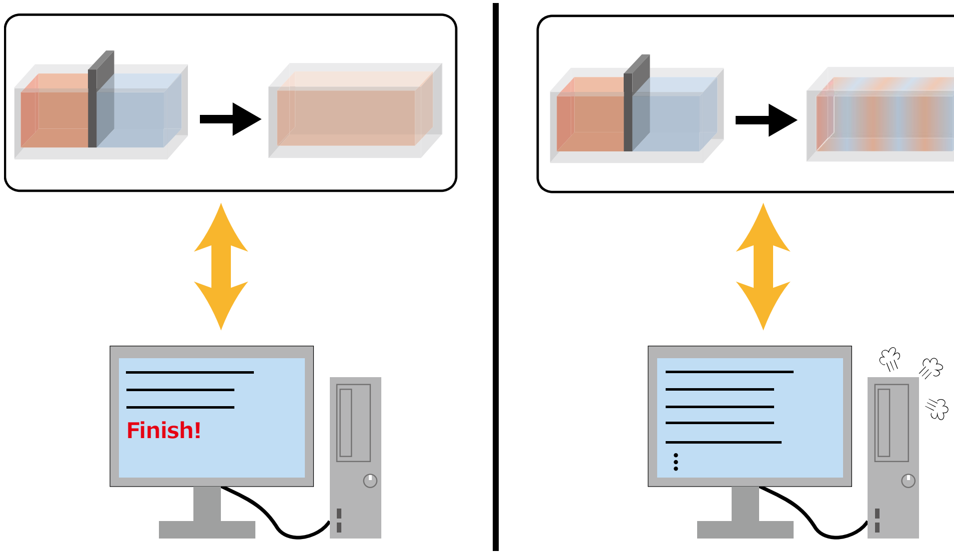
(Universal TM: a computer which can compute any computational task)

This problem is undecidable (There is no procedure deciding whether this TM halts or not).



Most important lemma

Lemma：For any program of universal TM, there exists a corresponding Hamiltonian such that it thermalizes iff the TM with this program halts.



Since halting problem is undecidable, thermalization is also undecidable.

Strategy

1. We first construct a proper **classical TM** which has different value of A between halting and non-halting of TM.

2. We **emulate** this classical system by quantum many-body systems. (Like Feynman-Kitaev construction)

Since 2 is a well known method, we mainly treat 1.

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Structure and dynamics

Two-layer structure

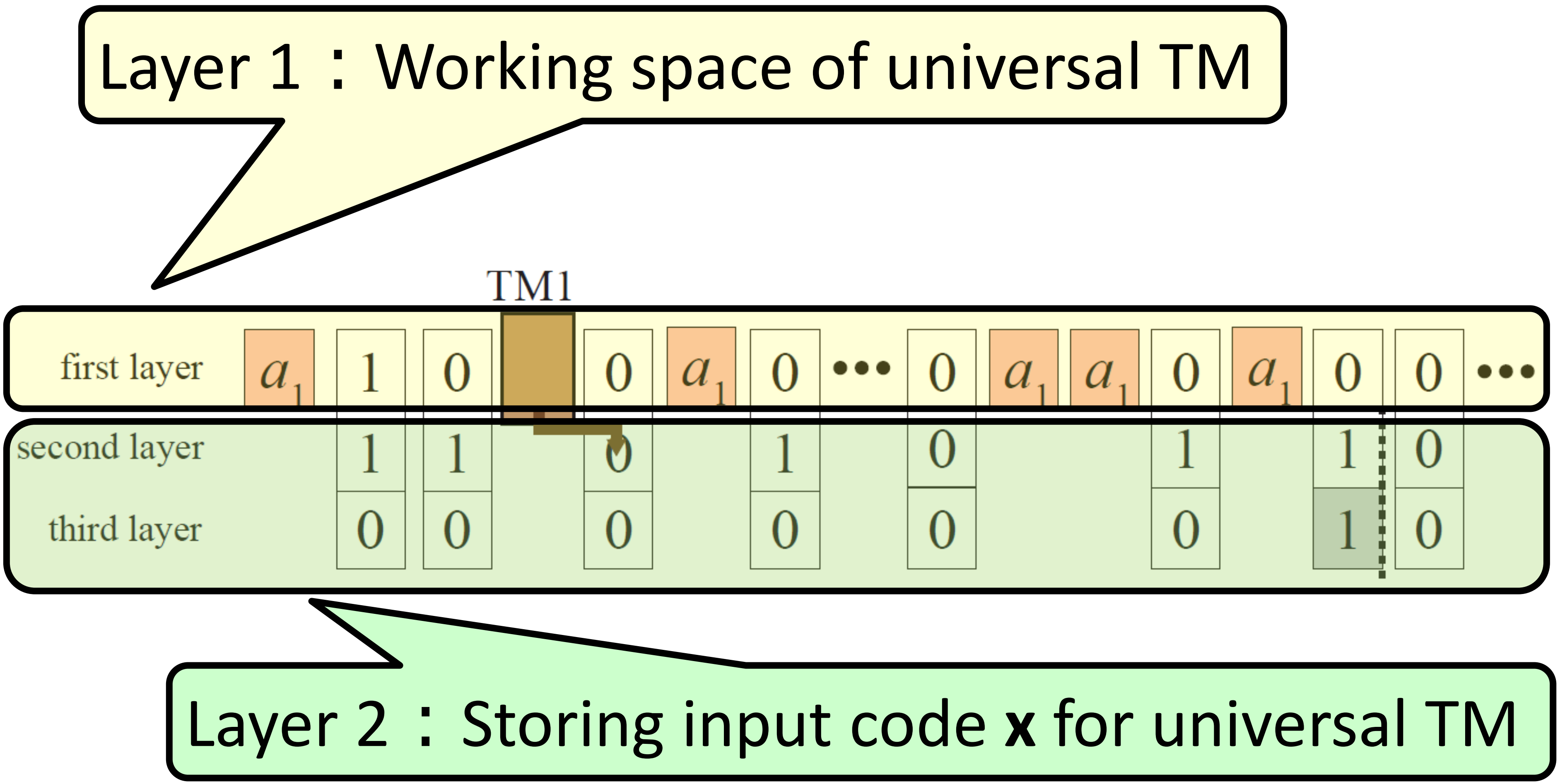
Layer 1 ： Working space of universal TM

Layer 2 ： Storing input code **x** of universal TM.

Dynamics

1. Decode input code **x** from Layer 2.
2. Universal TM runs with input code **x**.
3. Flip the value of observable A if and only if the universal TM halts.

Structure of classical TM (schematic)



Step 1: How to decode the input **x**

input x with 01 bit ↔ real number $\boldsymbol{\beta}$ in decimal

classical：Set the probability of bit 1 as β.

quantum：Align $\sqrt{\beta}|1\rangle + \sqrt{1-\beta}|0\rangle$.

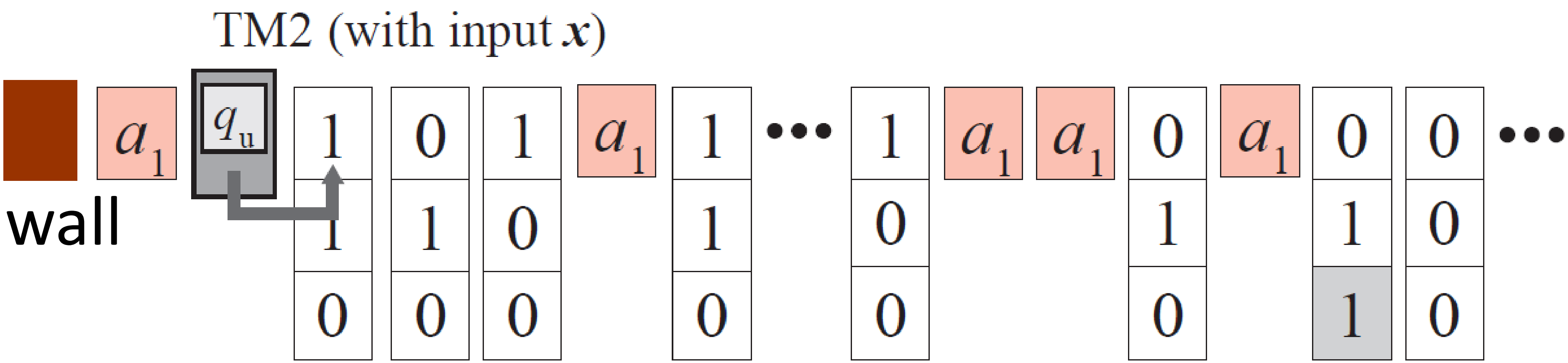
(ex: If input code is x=1101, $\beta = 0.1011 = \frac{1}{2} + \frac{1}{8} + \frac{1}{16} = \frac{11}{16}$)

•••	1	1	1	1	0	1	0	1	1	1	1	0	1	1	1	1	•••

TM1 estimates the **relative frequency of 1** in layer 2, and output the result to layer 1.

Step 2: in case of non-halting

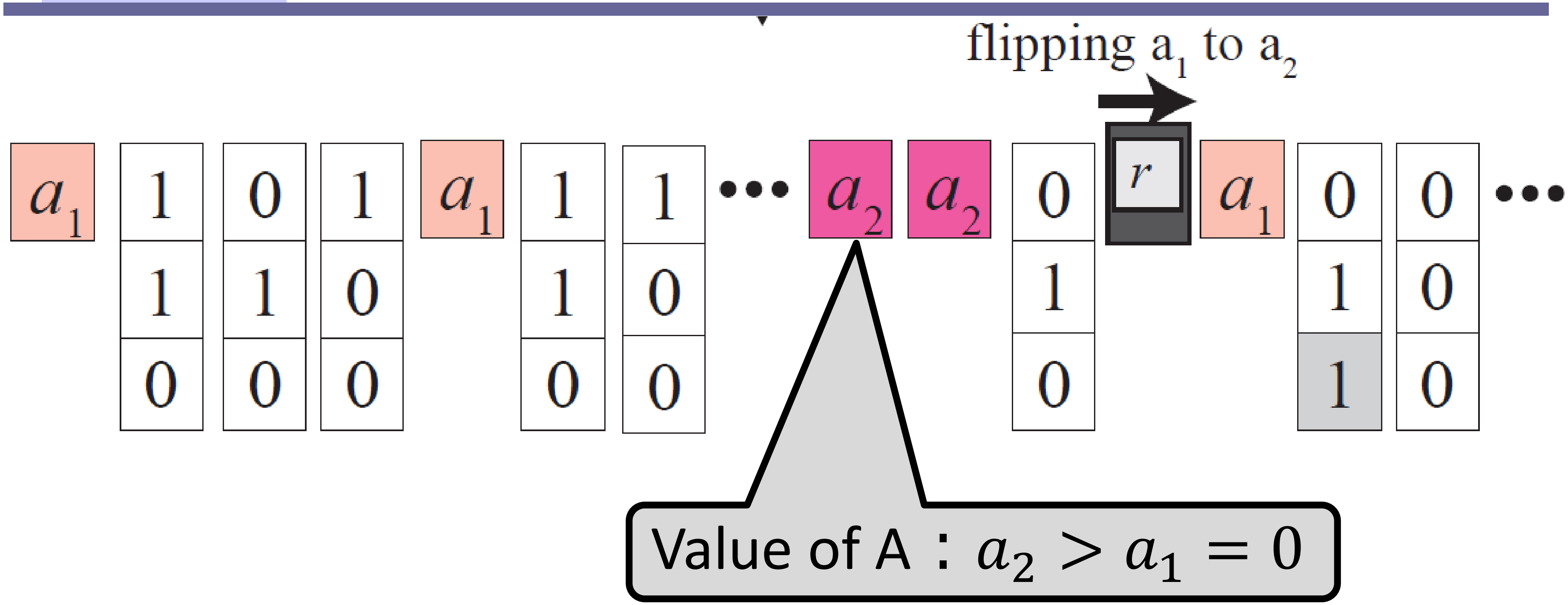
Universal TM runs with input **x.**



We set the L-th cell as "wall" at the first step.
If TM2 steps across the periodic boundary (wall), then TM2 stops.

In case of non-halting, TM2 must hit wall at some time.

Step 3: flipping (in case of halting)



(When all A-cells are flipped, TM3 stops (relaxation), or just spends time (thermalization))

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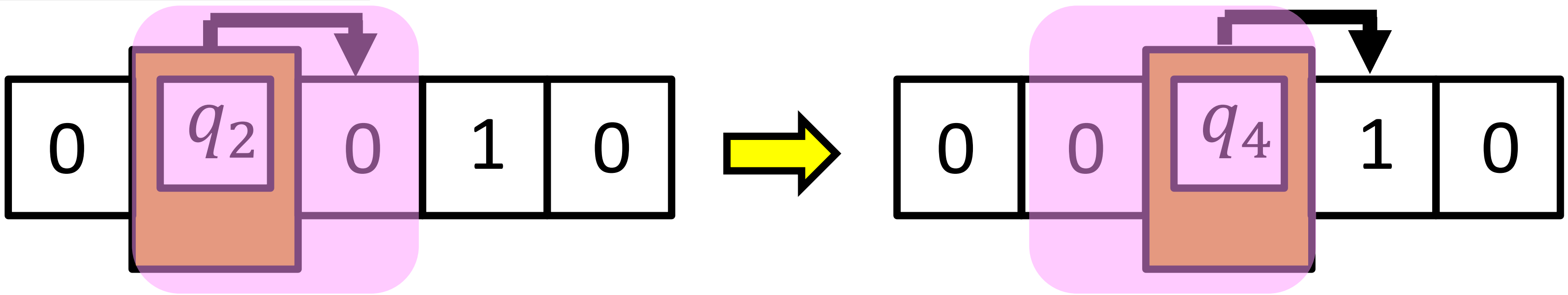
Feynman-Kitaev type Hamiltonian

<u>Classical TM</u>



<u>Quantum Hamiltonian</u>

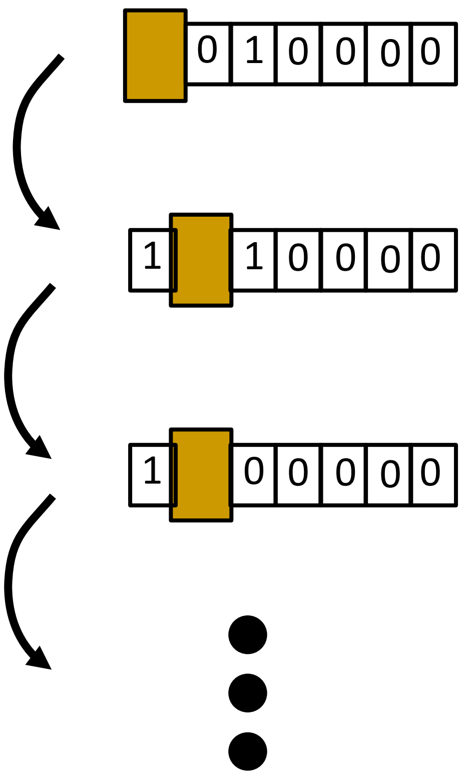
Local Hamiltonian should have $\mathbf{|0q_4\rangle\langle q_2 0| + c.c.}$.
(Total Hamiltonian has its shift-sum.)

- This Hamiltonian is **local** (nearest-neighbor).
- Only the vicinity of control unit can evolve.

Dynamics in classical system = Eigenstate in quantum system

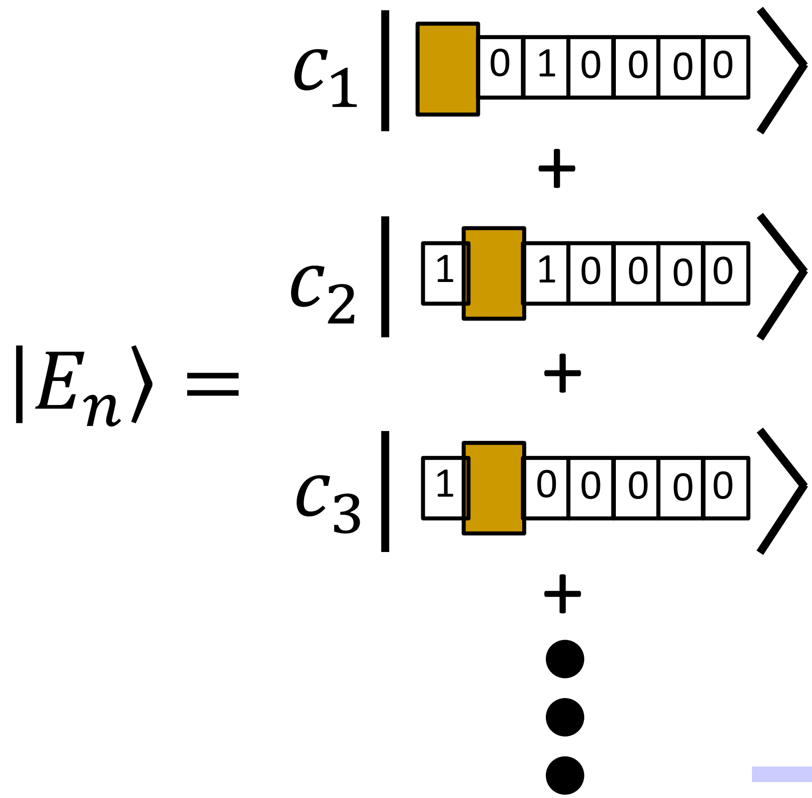
Classical system

Dynamics of CA



Quantum system

Single energy eigenstate



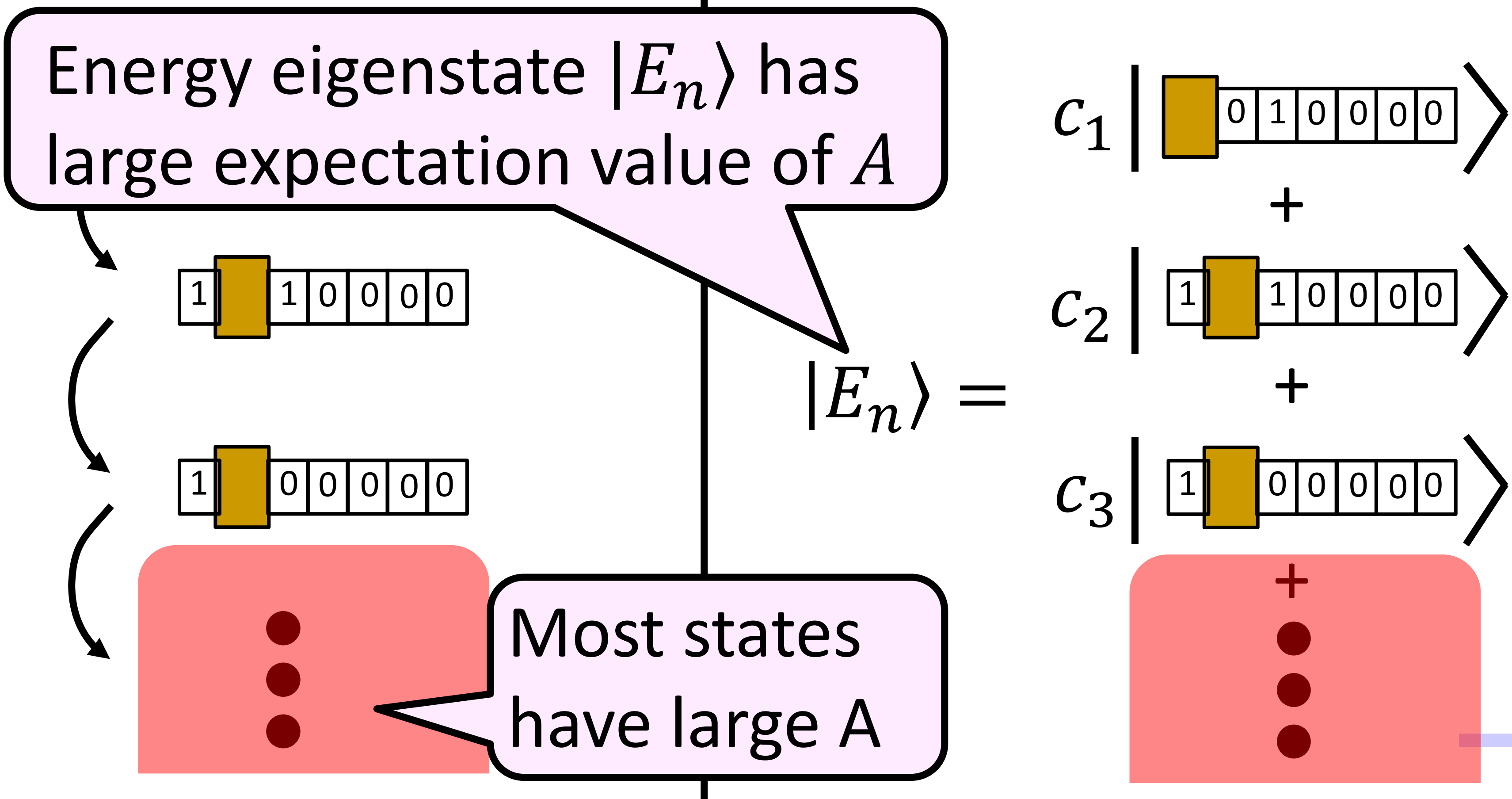
In case of halting...

Classical system

Dynamics of CA

Quantum system

Single energy eigenstate



Thermalization is Turing complete

Is our result negative?

Our result shows not only undecidability but also **Turing completeness** of thermalization.

Turing completeness $\simeq$ All possible computation

Any computational task can be implemented by thermalization phenomena.

Striking example

Fact: There exists a (744-state) TM which halts if and only if Riemann hypothesis is false.

(C. Calude and E. Calude, Comp. Sys. 18, 267. (2009)/ A. Yedidia and S. Aaronson, arXiv:1605.04343/ S. Aaronson, https://www.scottaaronson.com/papers/bb.pdf)

⬇

There exists a 1d system which thermalizes if and only if **Riemann hypothesis is false**.

(Though the fate of Riemann hypothesis is unknown at present, we can construct this Hamiltonian)

Summary of this talk

Part 1: General framework to violate ETH

We construct nonintegrable thermalizing system without ETH systematically. This is related to quantum many-body scars.

N. Shiraishi and T. Mori, Phys. Rev. Lett. 119, 030601 (2017)
T. Mori and N. Shiraishi, Phys. Rev. E 96, 022153 (2017)
N. Shiraishi, J. Stat. Mech. 083103 (2019)

Part 2: Undecidability of thermalization

Thermalization in a general form is proven to be undecidable problem.

N. Shiraishi and K. Matsumoto, Nat. Comm. 12, 5084 (2021)

END