Undecidability in quantum thermalization

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

Outline

Review of quantum thermalization

Review of theoretical computer science

Setup and main result

Proof – step 1: Construction of classical machine

Proof – step 2: Emulation by quantum system

Outlook

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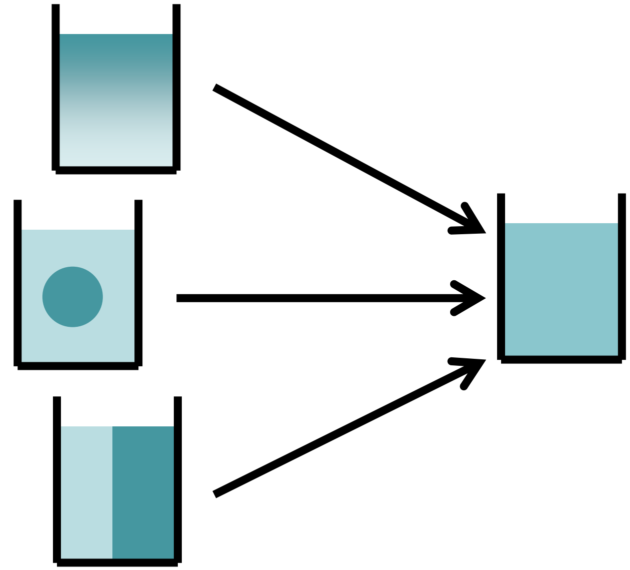
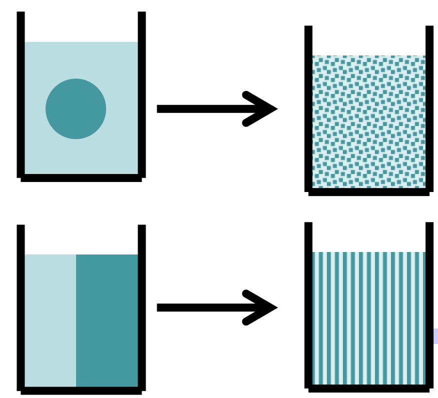
Thermalization of macroscopic system

Thermalization

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



But some systems **do not thermalize!**
(e.g., integrable systems)



Big problem:

- **What determines whether a system thermalizes or not?**
- **How to understand thermalization phenomena?**

What is thermal?

Def: Thermal

A state $|\psi\rangle$ is **thermal w.r.t.** $\boldsymbol{A}$ if

$$\langle\boldsymbol{\psi}|\boldsymbol{A}|\boldsymbol{\psi}\rangle \simeq \mathbf{Tr}[\boldsymbol{\rho}_{\boldsymbol{MC}}\boldsymbol{A}].$$

Here, ρ_{MC} is the microcanonical distribution with energy $\langle\psi|H|\psi\rangle$.

("$\simeq$" means that these two are equal in thermodynamic limit)

Typicality: Almost all pure states are thermal.

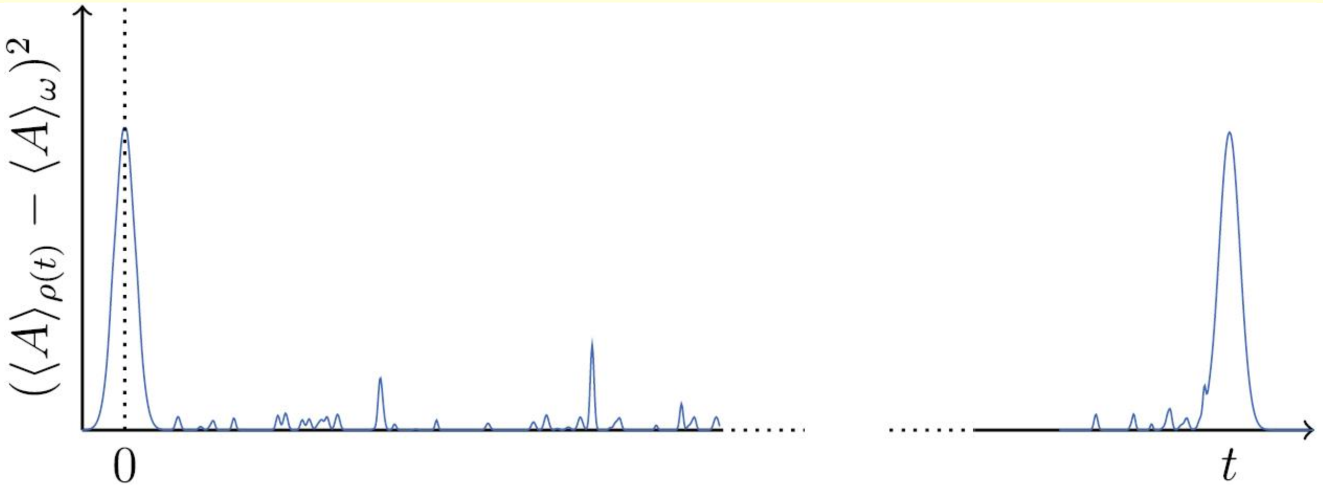
(S. Popescu, A. Short, A. Winter, Nat. Phys. 2, 754 (2006))

What is thermalization?

<u>Def: Thermalization</u>

A state $|\psi(0)\rangle$ thermalizes w.r.t. A if **for almost all t**, $|\psi(t)\rangle := e^{-iHt}|\psi(0)\rangle$ **is thermal w.r.t. A**.

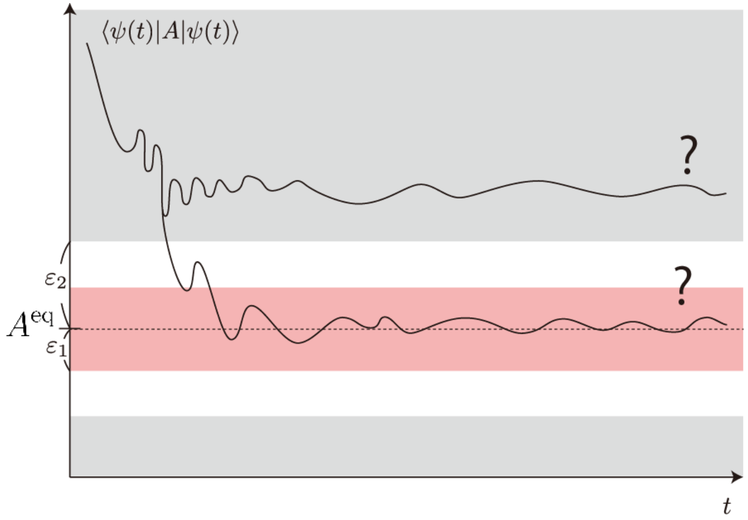
$$\lim_{T\to\infty}\frac{1}{T}\int_0^T dt\,\chi(|\psi(t)\rangle \text{ is thermal w.r.t. A}) \simeq 1$$



(C. Gogolin and J. Eisert, *Rep. Prog. Phys.* 79 056001 (2016))

Our target

We would like to know **whether an initial state $|\psi(0)\rangle$ with Hamiltonian H thermalizes or not w.r.t. an observable A**.



We show that this is **undecidable**.

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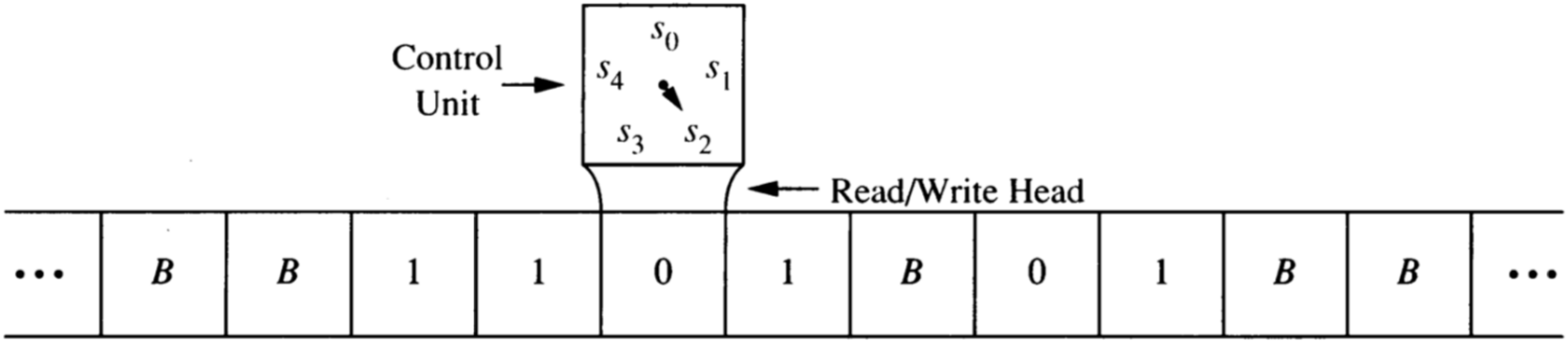
Computation by Turing machine

Turing machine (TM)



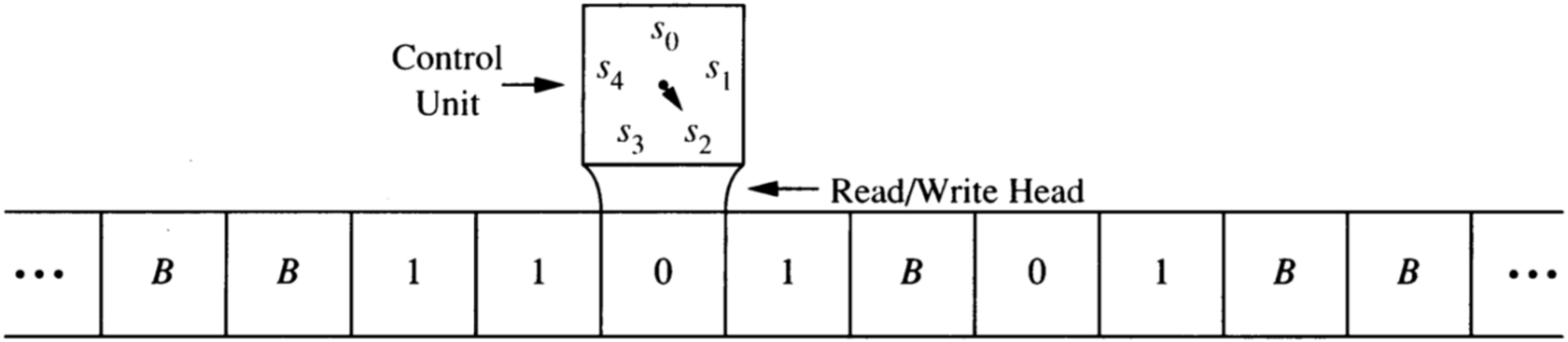
(https://rpruim.github.io/m252/S19/from-class/models-of-computation/turing-machines.html)

Control unit reads a single cell (with 0/1/Blank) and

- change its own internal state
- rewrite the state in the read cell
- move left/right one cell.

Computation by Turing machine

Turing machine (TM)



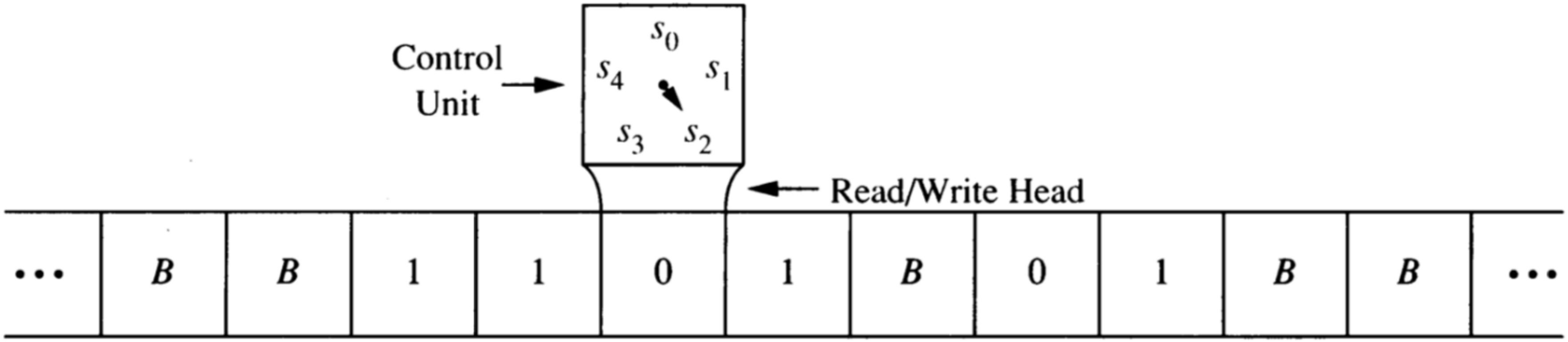
(https://rpruim.github.io/m252/S19/from-class/models-of-computation/turing-machines.html)

Ex of rule: If internal state is s_2 and head reads 0,

- Internal state is changed to s_4.
- The cell is kept at 0 (not rewritten).
- The head moves right.

Computation by Turing machine

Turing machine (TM)



(https://rpruim.github.io/m252/S19/from-class/models-of-computation/turing-machines.html)

Church-Turing thesis

Despite its simplicity, there exists **universal reversible TM (URTM)** which can emulate any computational task.

Decision problem

Def: Decision problem

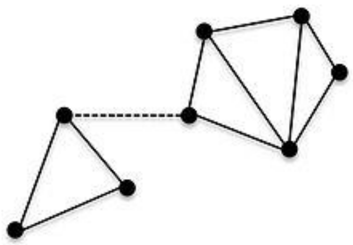
Yes-No question of input.

Ex) -Primality test

Input: A natural number N.

Problem: Is N prime?

-Graph connectivity test

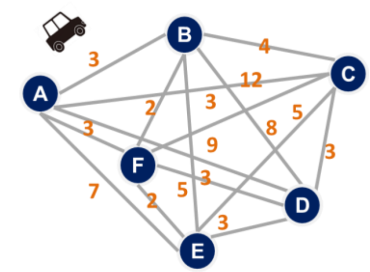


Input: A graph.

Problem: Are any two vertices connected?

Decidable/undecidable

<u>Def: 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

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

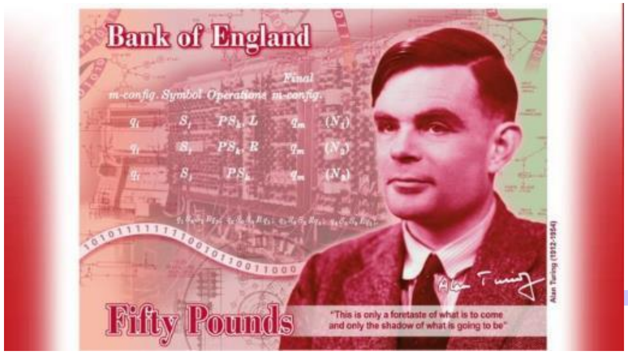
<u>Def: Undecidable</u>： There is no procedure/algorithm which decides Yes/No correctly for all inputs (Of course, there is no general theorem).

(Related to Godel’s incompleteness theorem)

Undecidability of halting problem

<u>Def: Halting problem of Turing machine</u>
<u>Input</u>: an input code for a fixed URTM.
<u>Problem</u>: Does URTM with this input "halt at some time" or "not halt forever"?

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



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Our system

System：1d system with periodic boundary condition

Dimension of local Hilbert space：d (fixed)

Observable A	Given arbitrarily and fixed
Initial state $\|\psi(0)\rangle$	Given arbitrarily and fixed
Hamiltonian H	Input

Complicated $A, |\psi(0)\rangle, H$ make the decision problem hard.
However, we show that even with **simple** $\boldsymbol{A}, |\boldsymbol{\psi}(\mathbf{0})\rangle, \boldsymbol{H}$, thermalization is undecidable.

Statement of decision problem

Arbitrarily given parameters

Observable：spatial average of 1-body observable

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

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 $\boldsymbol{H} = \sum_{\boldsymbol{i}} \boldsymbol{h}_{\boldsymbol{i},\boldsymbol{i}+\mathbf{1}}$

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

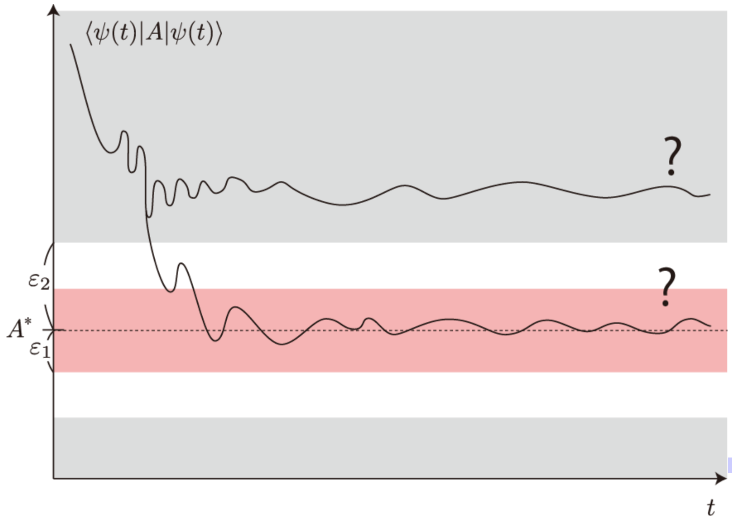
Statement of decision problem

<u>Decision problem of relaxation with promise</u>

Decide whether the difference between

- $\bar{A}$ (long time average of A)
- a given value A^*

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

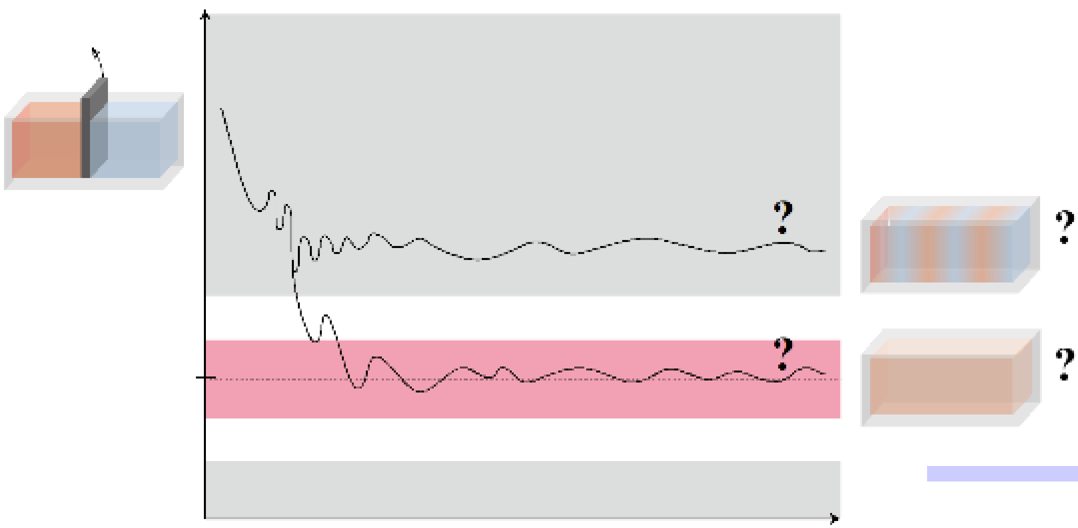


Main result: Undecidability in thermalization

Theorem：For any $A, |\psi(0)\rangle$, decision problem of thermalization (with promise) is **undecidable**. (No algorithm decides the presence/absence of thermalization for a given Hamiltonian)

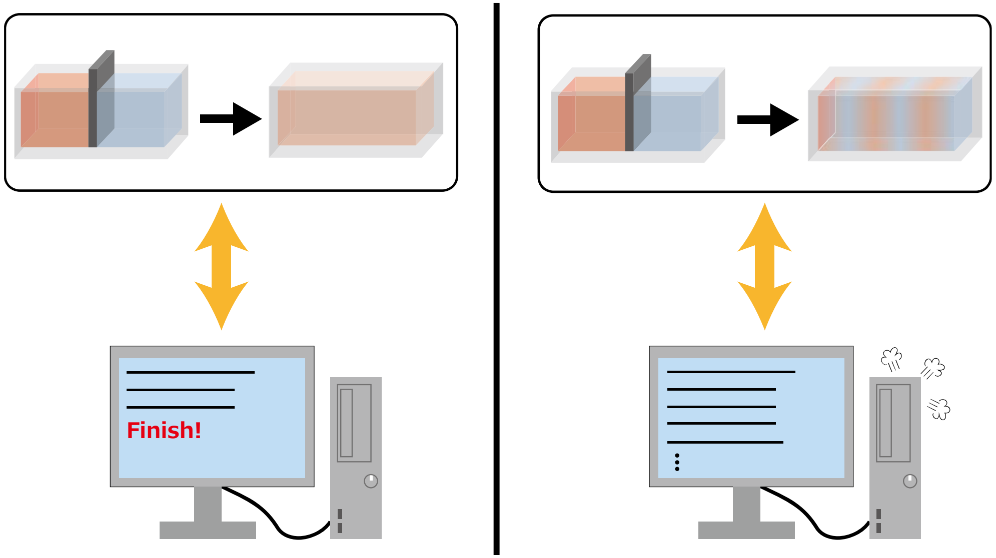
(NS and K. Matsumoto, Nat. Comm. 12, 5084 (2021))

(Since it is easy to A^* to the equilibrium value A_{eq}, we show the undecidability of relaxation in the following.)



Important lemma

Lemma：For any code for URTM, there exists a corresponding Hamiltonian such that the system thermalizes iff URTM with this code halts.



Since the halting problem is undecidable, thermalization is also undecidable.

Proof outline of the lemma

1. Construct a classical many-body system (cellular automata: CA) whose long-time average of A varies depending on whether the URTM with the corresponding code halts or not.

2. Emulate this classical dynamics by a quantum many-body system (Feynman-Kitaev construction)

Since 2 is a well-known method, we mainly treat 1 in the following.

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Structure of states of classical CA

There are two types of cells:

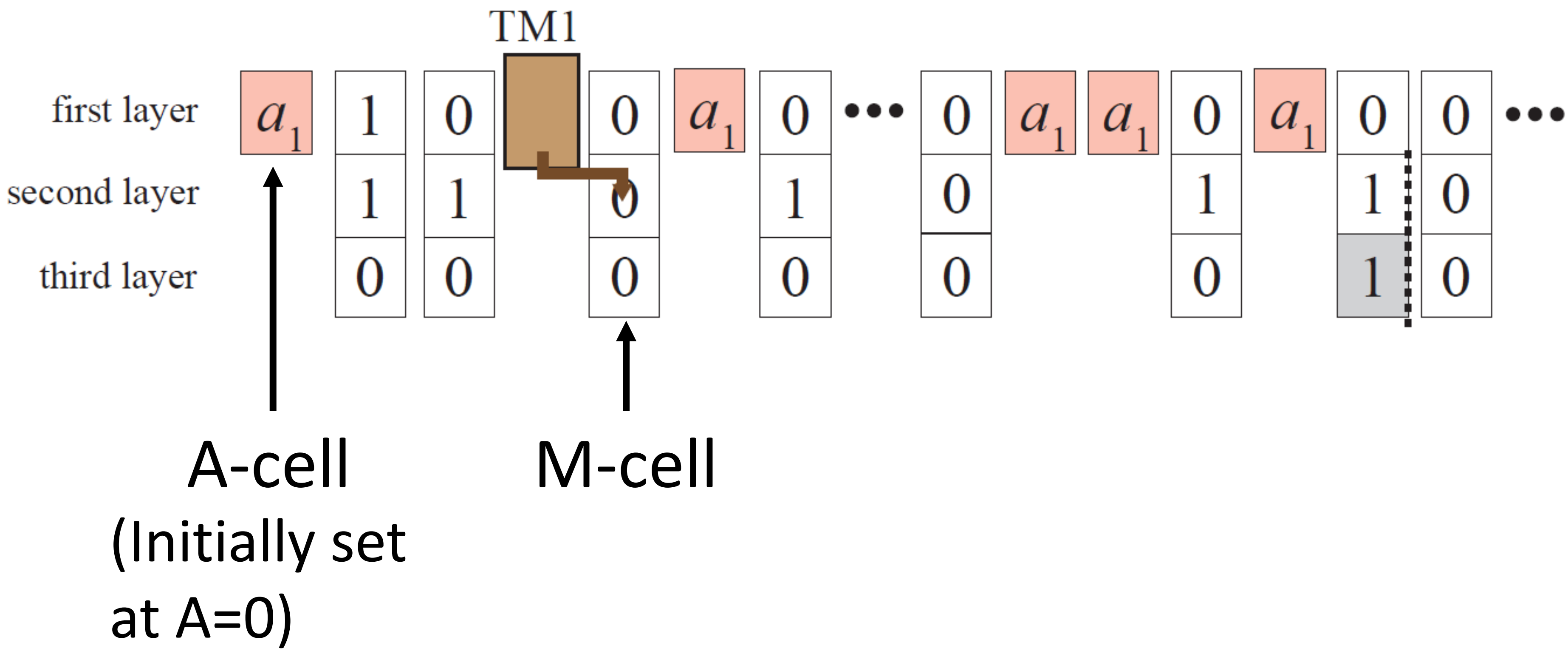
M-cells: - storing the input code for URTM
- a working space of URTM.

M-cell consists of three layers.

A-cells: - change the value of A between the case of halting and non-halting.

Three Turing machines, TM1 and TM2 (in M-cells), and TM3 (in A-cells) run in these cells.

State of total system (with computational basis state)



When TM moves, the cell and finite control are swapped. Otherwise, the type of cells are kept.

Structure of M-cell

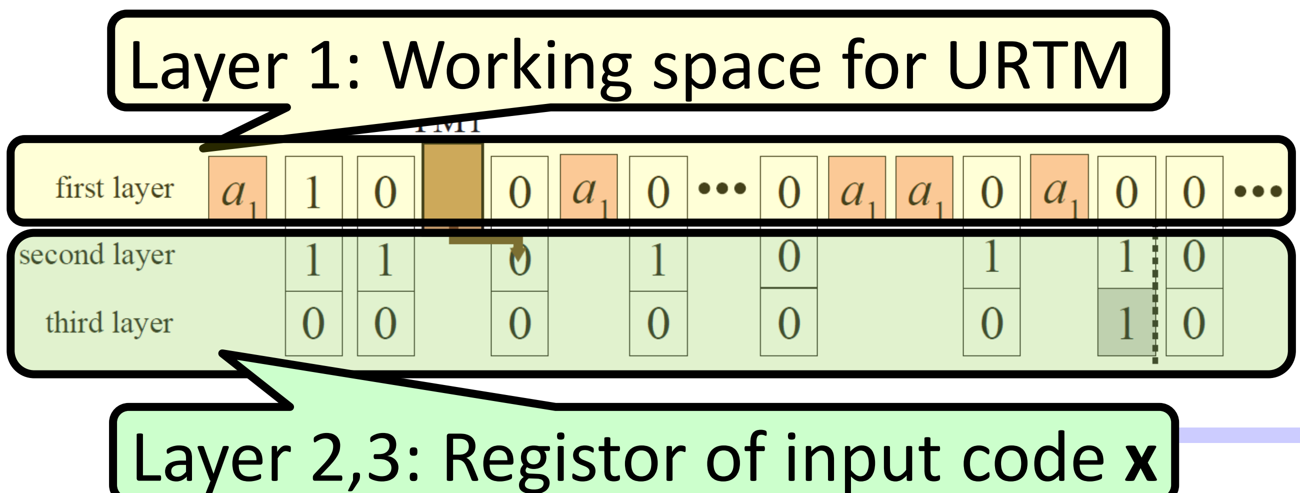
M-cell consists of 3 layers:

Layer 1 : emulate classical URTM (input **x**)

Layer 2 : spin 1/2

Layer 3 : spin 1/2

(Layers 2 and 3) possess information of input bit sequence **x** for URTM



Whole dynamics (forward direction)

TM1 decodes input code **x** from layers 2,3.

↓

TM2 (URTM) runs with input code **x**

not halt → Nothing happens (**A is zero**)

halts → TM3 flips states of A-cells (**A becomes finite**)

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

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

Classical：Set β to the frequency of bit 1

Quantum：Line up the state $\sqrt{\beta}|1\rangle + \sqrt{1-\beta}|0\rangle$

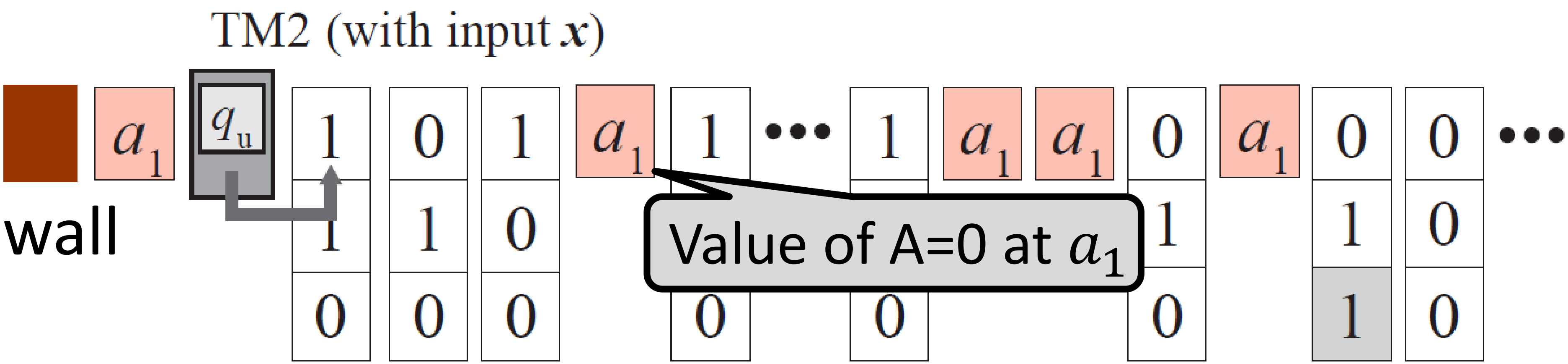
(ex: When input code is x=1101, $\beta = 0.1011 = \frac{1}{2} + \frac{1}{8} + \frac{1}{16} = \frac{11}{16}$)

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

Measure the relative frequency of 1 in layer 2, and output it to layer 1.

Step 2: Before halting

TM2 (URTM) runs with input **x**.

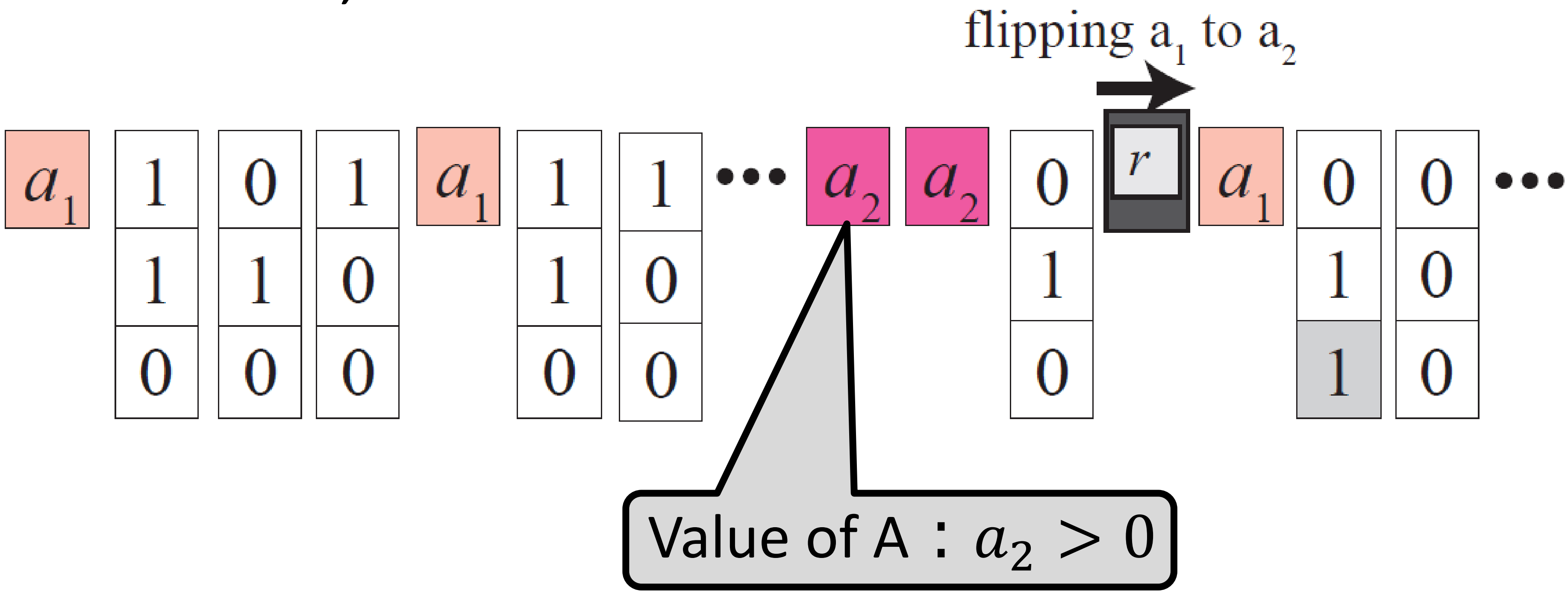


If TM2 steps across the periodic boundary, then TM2 stops (We set the L-th cell as “wall” and TM2 stops when it hits the wall).

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

Step 3: flipping

If TM2 halts,...



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

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Structure of Hamiltonian

Basic structure ： Feynman-Kitaev Hamiltonian (without clock)

Hamiltonian is written as $H = V + V^\dagger$

move one step forward

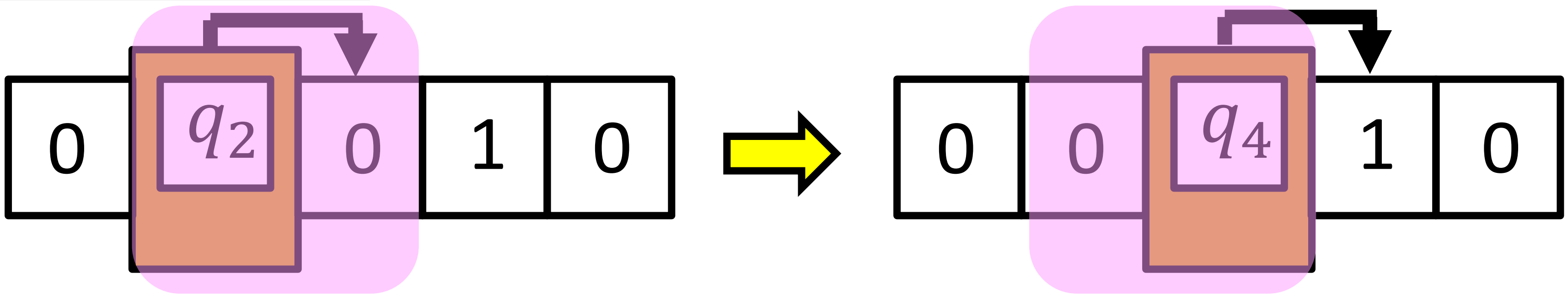
move one step backward

$$V|\boldsymbol{x}^n\rangle = |\boldsymbol{x}^{n+1}\rangle, \qquad V^\dagger|\boldsymbol{x}^n\rangle = |\boldsymbol{x}^{n-1}\rangle$$

($|\boldsymbol{x}^n\rangle$: state of classical TM at n-th step)

Example of Feynman-Kitaev type Hamiltonian

Classical TM



Quantum Hamiltonian

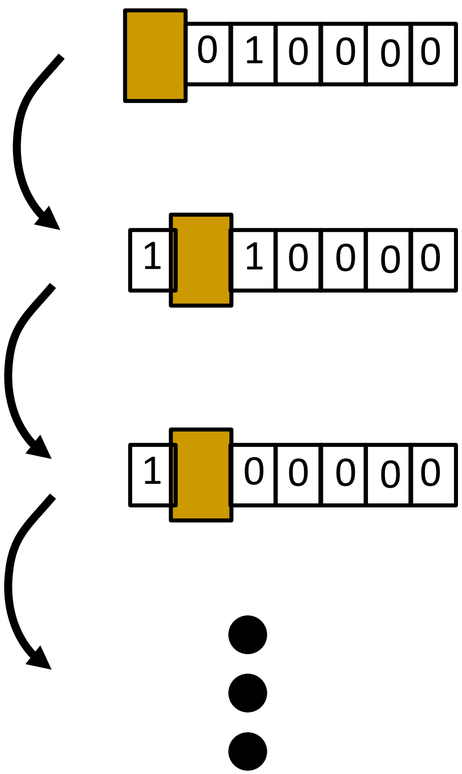
Local Hamiltonian should have $|\mathbf{0}\boldsymbol{q_4}\rangle\langle\boldsymbol{q_2}\mathbf{0}| + \boldsymbol{c}.\boldsymbol{c}.$.
(Total Hamiltonian has its shift-sum.)

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

Dynamics in classical system = Eigenstate in quantum system

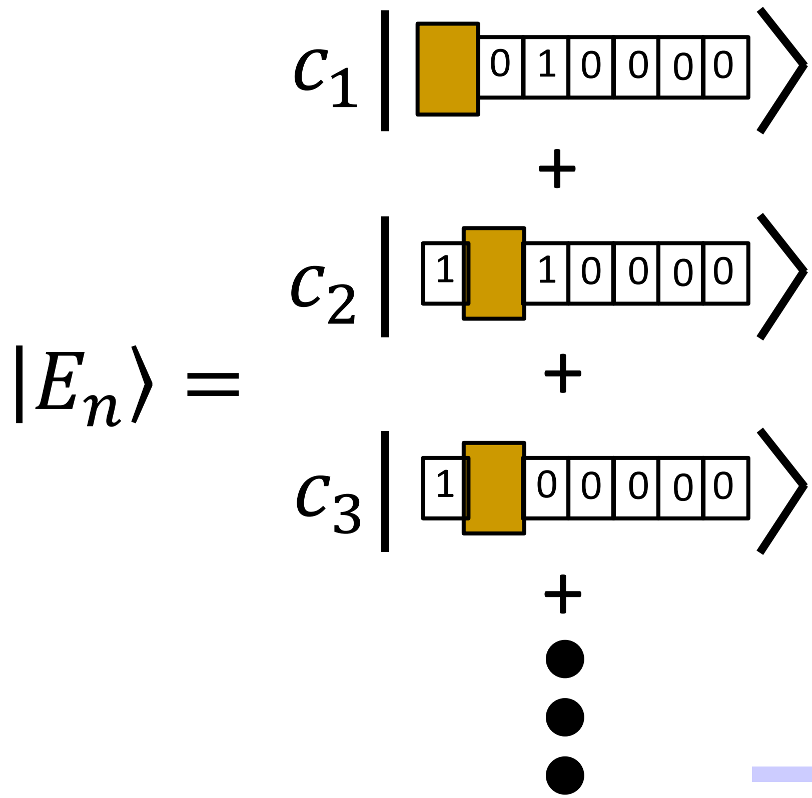
Classical system

Dynamics of CA



Quantum system

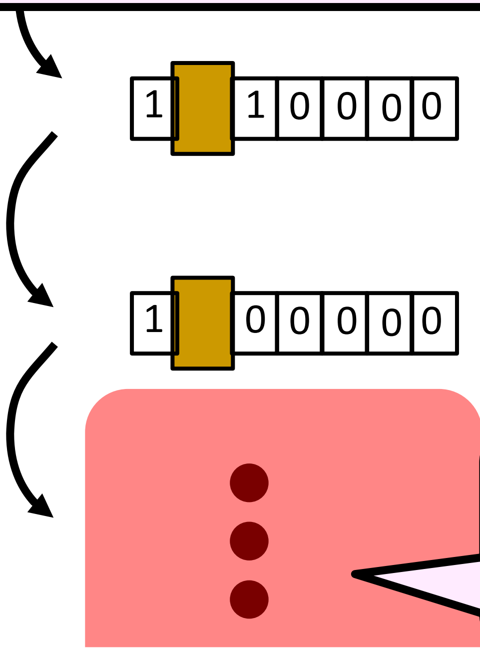
Single energy eigenstate



In case of halting…

Classical system

Dynamics of CA

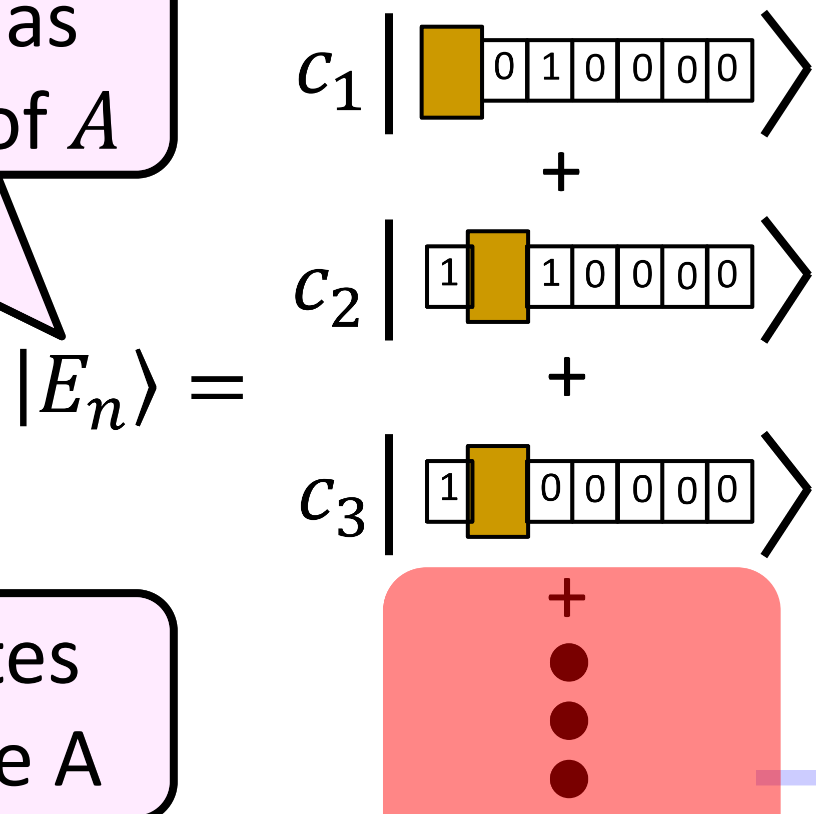


Energy eigenstate $|E_n\rangle$ has large expectation value of A

Most states have large A

Quantum system

Single energy eigenstate



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Thermalization is Turing complete

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**.

(Note: Step 1 (decoding) is unnecessary.)

Summary

- In the most general form, problem of thermalization is undecidable (unsolvable).
- This undecidability remains even for shift-invariant nearest-neighbor interactions system with one-body operators.
- Thermalization is Turing complete, which implies that thermalization is much more complicated phenomena than expected.

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

END