Undecidability in quantum thermalization

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N. Shiraishi and K. Matsumoto,
arXiv:2012.13889/arXiv:2012.13890 (accepted to Nat. Comm)

Outline

Background

Review of theoretical computer science

Main result

- Setup and main claim
- Constructing classical Turing machine
- Constructing quantum system
- Extension

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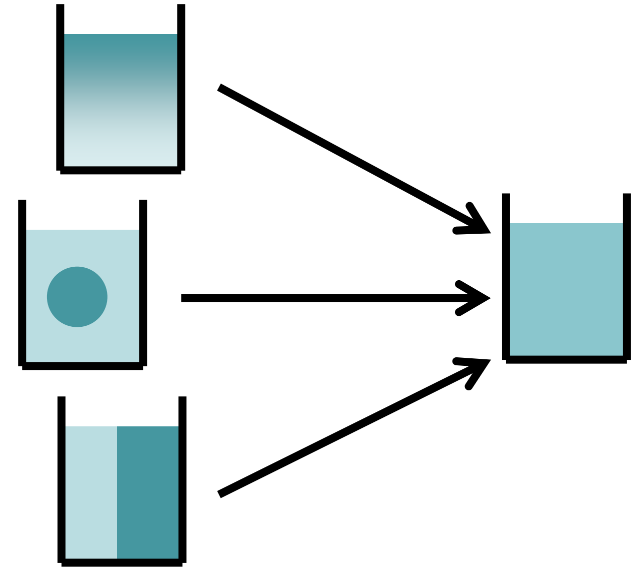
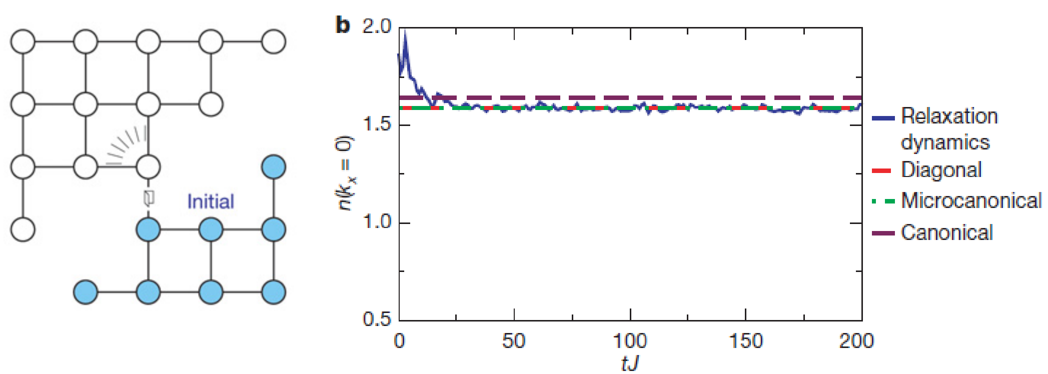
Thermalization of macroscopic system

<u>Thermalization</u>
Non-equilibrium state goes to a unique equilibrium state (i.e., macroscopically indistinguishable).



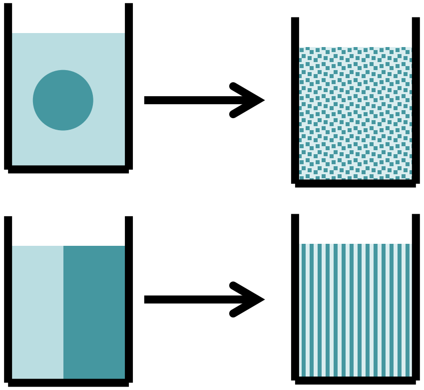
It is true for a macro **pure quantum state**.



(M. Rigol, V. Dunjko & M. Olshanii, Nature **452**, 854 (2008))

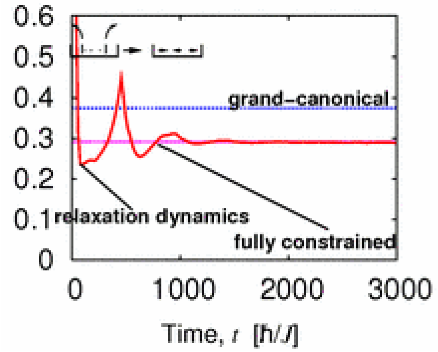
Why some systems thermalize while some others do not?

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



Ex) Integrable system

- Free Fermion system
- Bethe anzats (e.g., XXZ chain)



(M. Rigol, V. Dunjko, V. Yurovsky, and M. Olshanii, Phys. Rev. Lett. 98, 050405 (2007))

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

What is thermal?

Def: Thermal

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

$$\boldsymbol{\langle\psi|A|\psi\rangle \simeq \mathrm{Tr}[\rho_{MC}A]}.$$

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

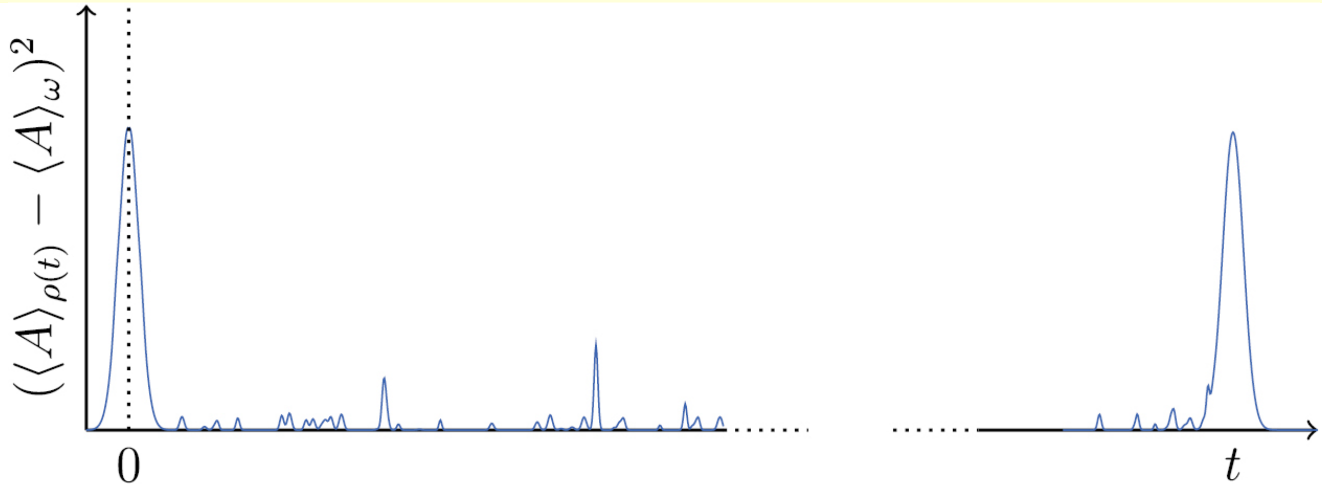
("$\simeq$" means that these two are equal in thermodynamic limit)

What is thermalization?

<u>Def: Thermalization</u>

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

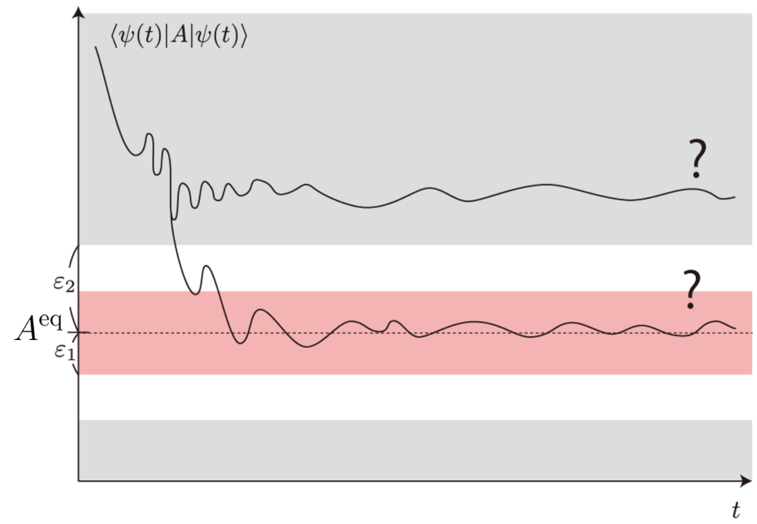
$$\lim_{T\to\infty}\frac{1}{T}\int_0^T dt\,\chi(|\psi(t)\rangle \text{ is thermal w.r.t. A}) \simeq 1$$



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

Our target

We would like to decide **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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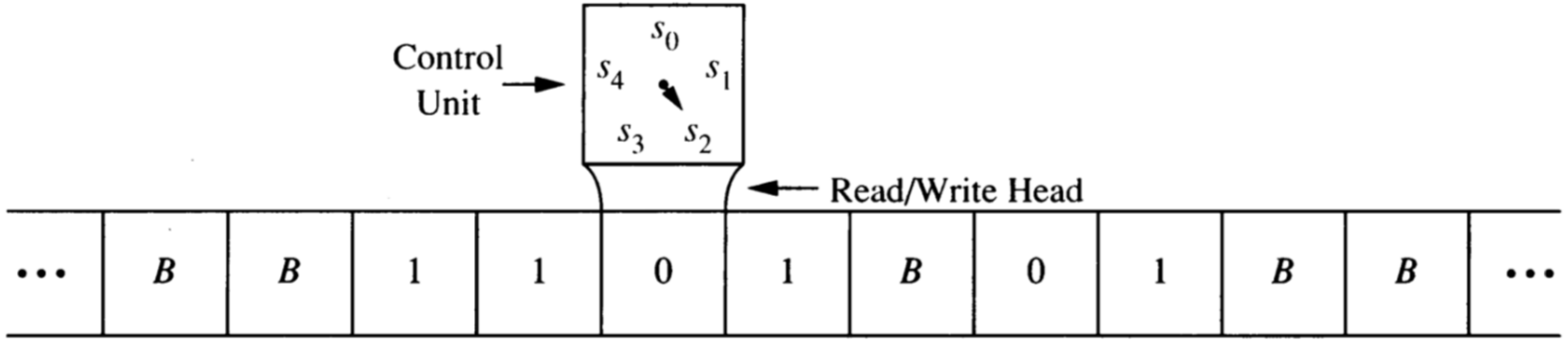
Computation by Turing machine

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 of the cell
- move left/right one cell.

What is computation?

There exists **universal reversible TM (URTM)** which can emulate any possible TM.

URTM can emulate almost all our computation system (e.g., C++/Python).

Church-Turing thesis

We identify computational functions as those computable by URTM.

computable = what TM can compute

Decision problem

Def: Decision problem

Yes-No question of input.

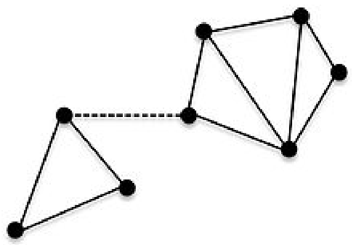
Ex) -Primality test

Input: A natural number N.

Problem: Is N prime?

-Graph connectivity test

Input: A graph.



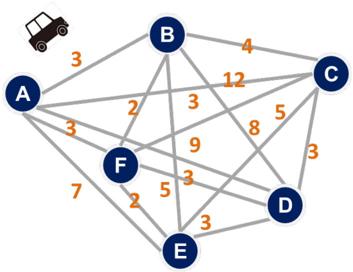
Problem: Are any two vertices connected?

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

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

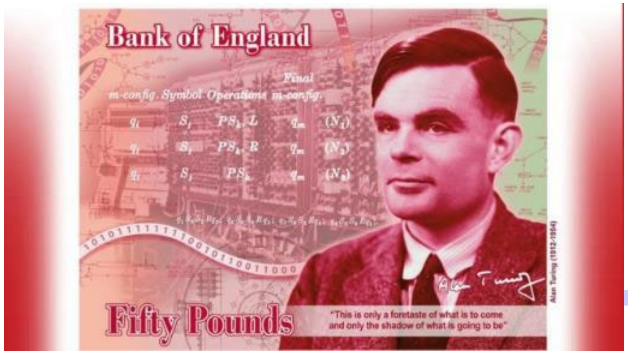
Def: Undecidable ： There is no procedure/algorithm which decides Yes/No correctly for all inputs (Of course, there is no general theorem).

(Related to Godel’s incompleteness theorem)

Undecidability of halting problem

<u>Def: Halting problem of Turing machine</u>
<u>Input</u>: an input 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 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

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

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.)

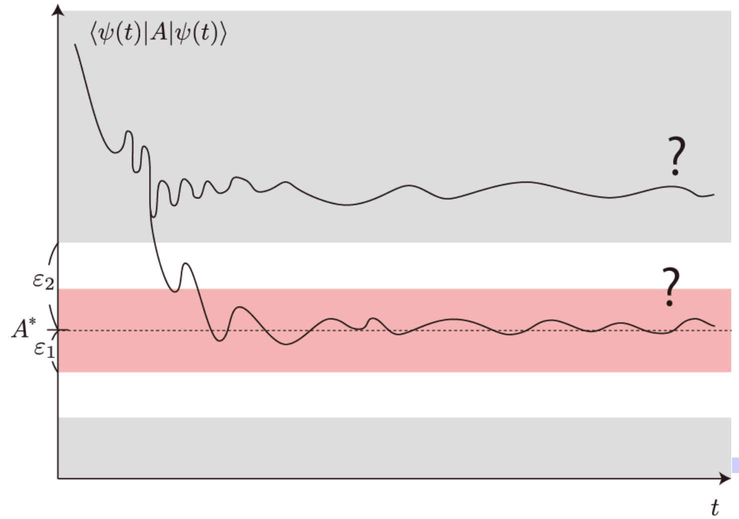
Statement of decision problem

<u>Decision problem with promise</u>

Decide whether the difference between

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

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



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

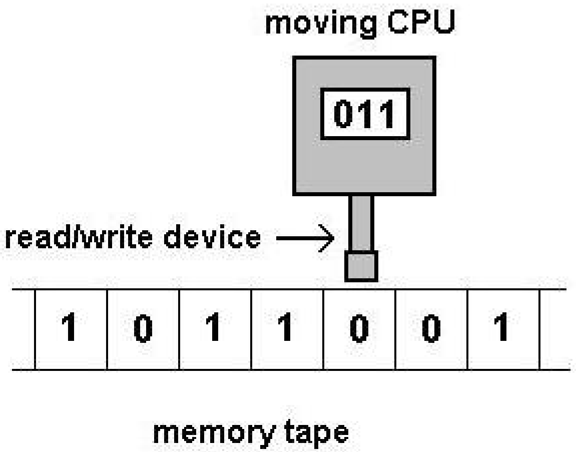
Proof idea: Reduction

<u>Proof sketch of undecidability of thermalization</u>

We homologize dynamics of the system to the halting problem of Turing machine (TM) as

not halt	**→**	**not thermalize**
halt	**→**	**thermalize**

Precisely, we prove that thermalization phenomena is computationally universal.



Strategy

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

2. We **emulate** this classical system by quantum many-body systems.

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Structure of states of classical TM

There are two types of cells:

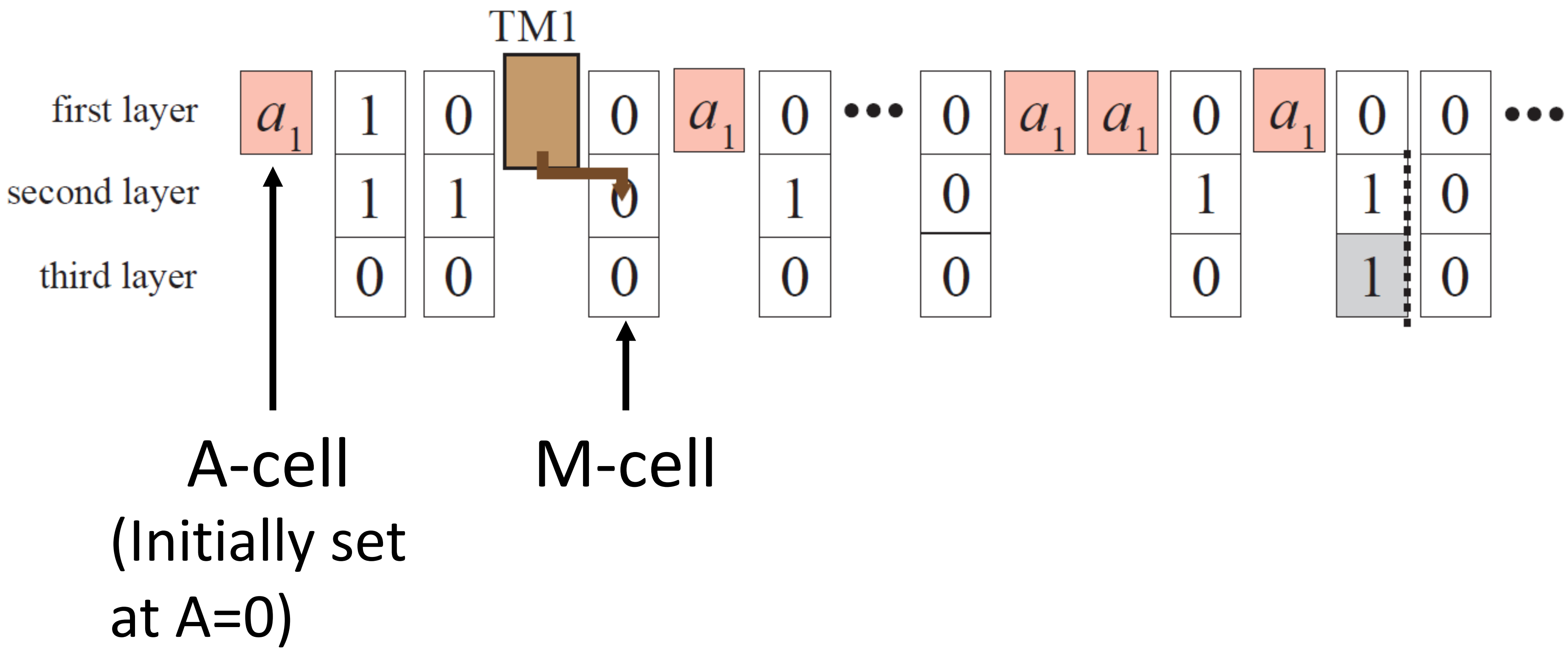
<u>M-cells</u>: - storing the input code for URTM
- a working space of URTM.

M-cell consists of three layers.

<u>A-cells</u>: - 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 cells might be swapped.
Otherwise, the type of cells are kept.

Structure of M-cell

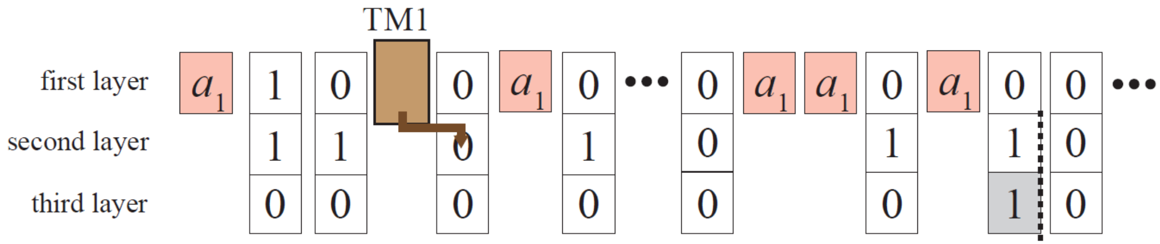
M-cell consists of 3 layers:

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

Layer 2：spin 1/2

Layer 3：spin 1/2

possess information of input bit sequence **x** for URTM



Whole dynamics (forward direction)

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

↓

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

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

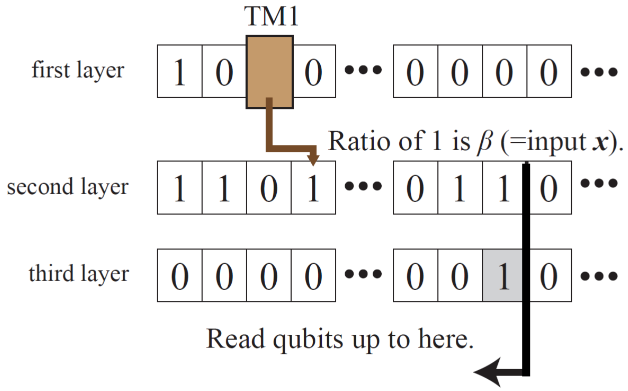
halts → TM3 flips states of A-cells (**A becomes finite**)

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

input x with 01 bit ↔real number β in decimal

We set relative frequency of 1 in layer 2 as β:

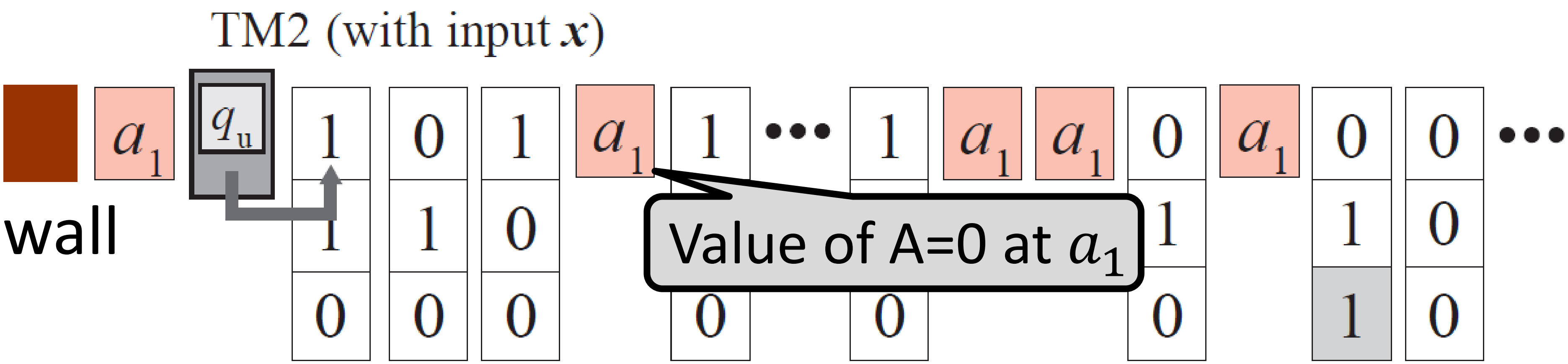
TM1 estimates the **relative frequency of 1** in layer 2, and output the result to layer 1.



Layer 3 determines how many bits TM1 should read and how many digits TM1 should output.

Step 2: Before halting

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

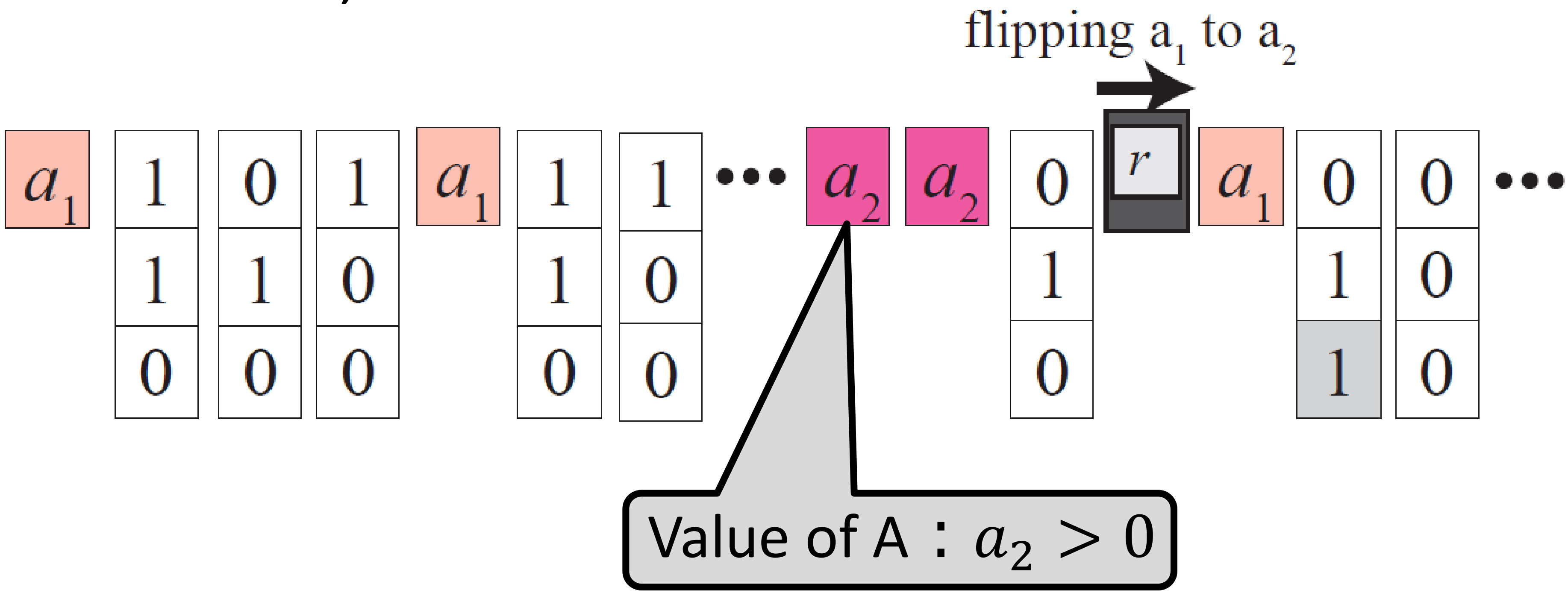


If TM2 steps across the periodic boundary, then TM2 stops (We set the L-th cell as “wall” and TM2 stops when it hits the wall).

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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Hamiltonian is input $\leftrightarrow$ state is input

<u>Original problem</u>

State is fixed at $|\phi_0\rangle \otimes |\phi_1\rangle \otimes |\phi_1\rangle \otimes \cdots \otimes |\phi_1\rangle$.

Local Hamiltonian is input.

1-site local unitary transformation

<u>Modified problem</u>

Local Hamiltonian is fixed at proper one.

State $|\psi_0\rangle \otimes |\psi_1\rangle \otimes |\psi_1\rangle \otimes \cdots \otimes |\psi_1\rangle$ is input.

Structure of Hamiltonian

Basic structure ： Feynman-Kitaev Hamiltonian (without clock)

Dynamics of classical TM

state $P \rightarrow$ state Q

Quantum Hamiltonian

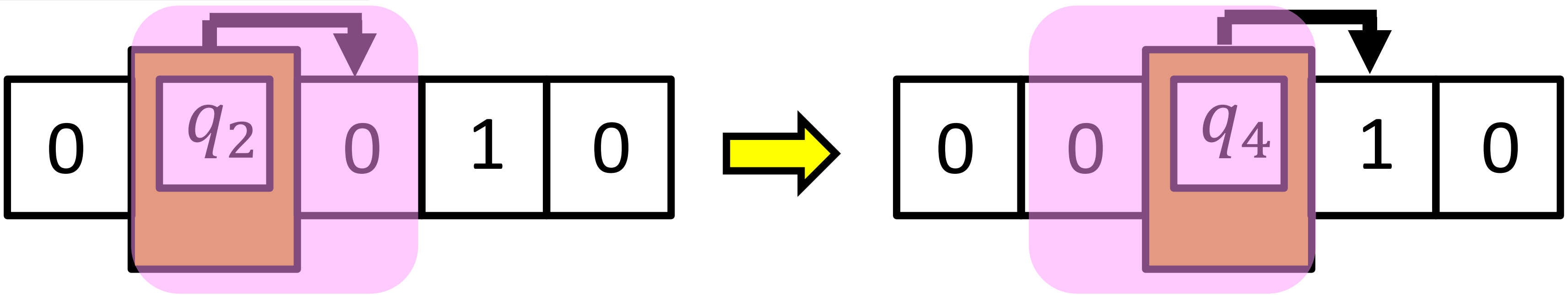
$|Q\rangle\langle P| + c.c.$

forward

backward

Example of Feynman-Kitaev type Hamiltonian

Classical TM



Quantum Hamiltonian

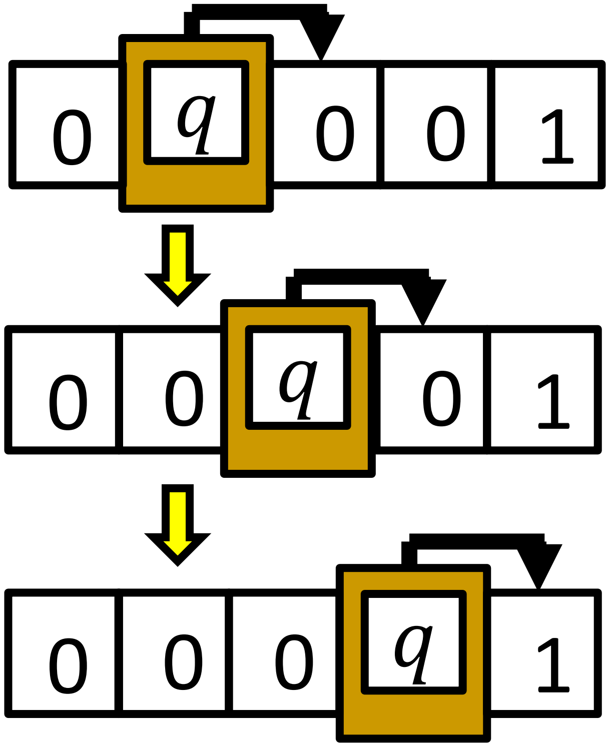
Local Hamiltonian should have $|\mathbf{0}\boldsymbol{q_4}\rangle\langle\boldsymbol{q_2}\mathbf{0}| + \boldsymbol{c.c.}$.
(Total Hamiltonian has its shift-sum.)

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

Further example of Feynman-Kitaev Hamiltonian

<u>Rule of classical machine</u>

- Internal state is unique, denoted by q.
- If TM reads 0, then it moves right.
- If TM reads 1, then it stops.



$$|0q001\rangle = |\boldsymbol{x}^1\rangle$$

$$|00q01\rangle = |\boldsymbol{x}^2\rangle$$

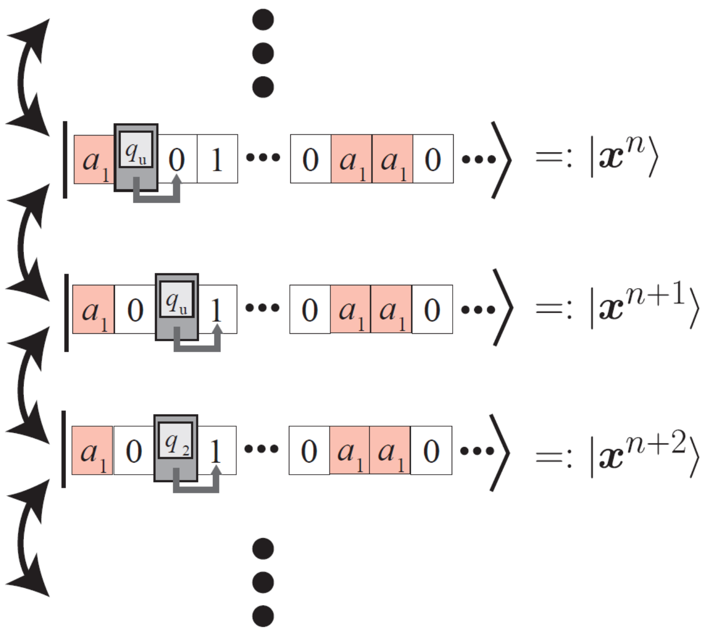
$$|000q1\rangle = |\boldsymbol{x}^3\rangle$$

Structure of Hamiltonian: after solving the classical dynamics

Denoting n-th state of the TM by $|\boldsymbol{x}^n\rangle$, we have effective description of Hamiltonian as

$$H = \sum_n |\boldsymbol{x}^{n+1}\rangle\langle\boldsymbol{x}^n| + c.c.$$

All energy eigenstates are **solvable** because this Hamiltonian is same as one-particle 1d lattice system with closed boundary condition.



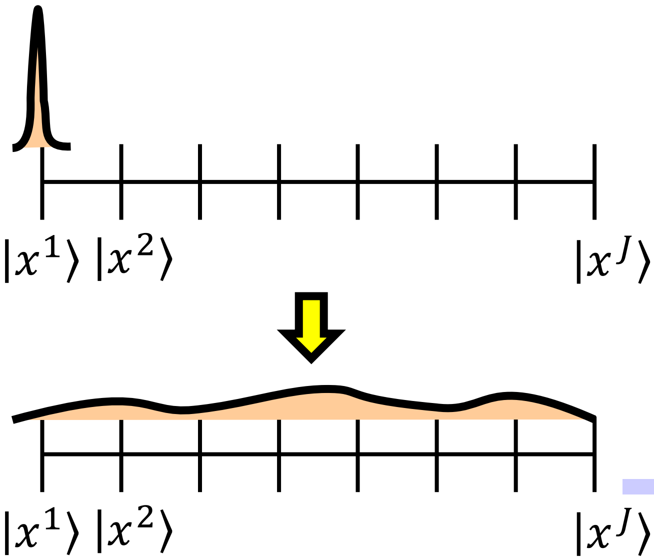
Exact energy eigenstates

$$E_j = 2\cos\left(\frac{j\pi}{J+1}\right)$$

$$|E_j\rangle = \sqrt{\frac{2}{J+1}}\sum_{k=1}^{J}\sin\left(\frac{kj\pi}{J+2}\right)|\boldsymbol{x}^k\rangle \qquad (1 \le j \le J)$$

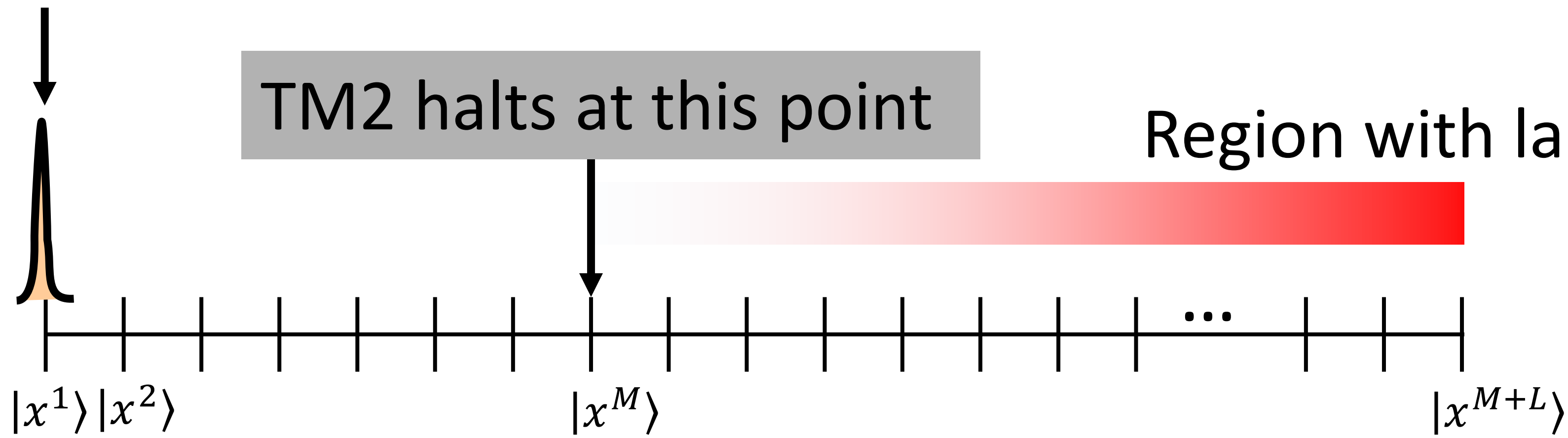
(J :number of steps before stopping the machine)

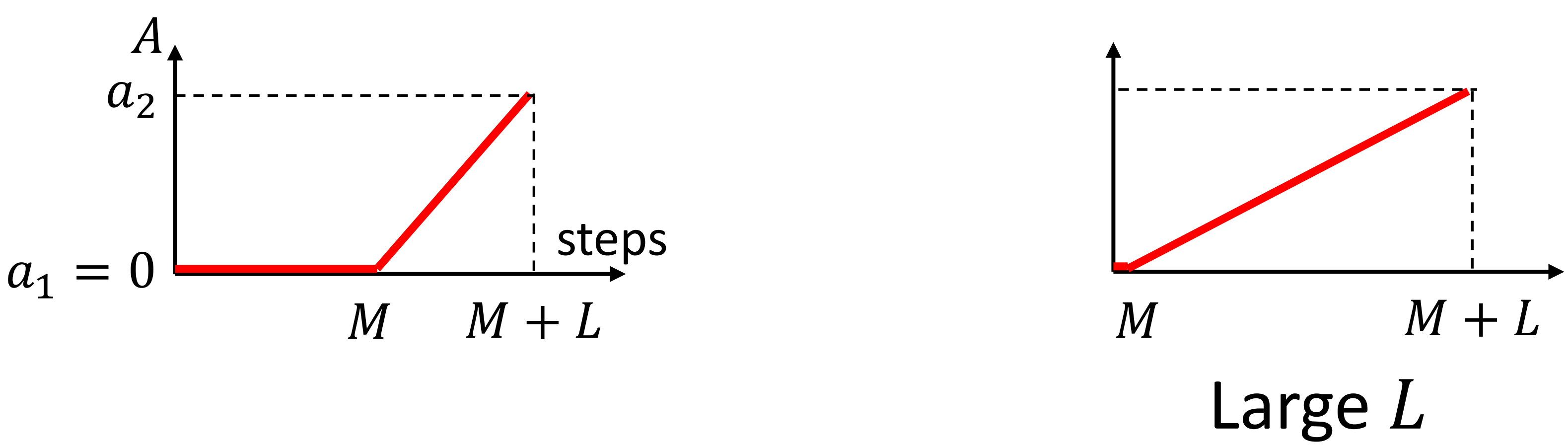
<u>Remark:</u> The quantum dynamics does *not* follow classical one directly. But, all states are in the **subspace spanned by** $\{\,|\boldsymbol{x}^1\rangle, \ldots, |\boldsymbol{x}^J\rangle\}$.



Quantum state space when TM2 halts (one-particle 1d description)

Localized at $|x^1\rangle$ when $t = 0$

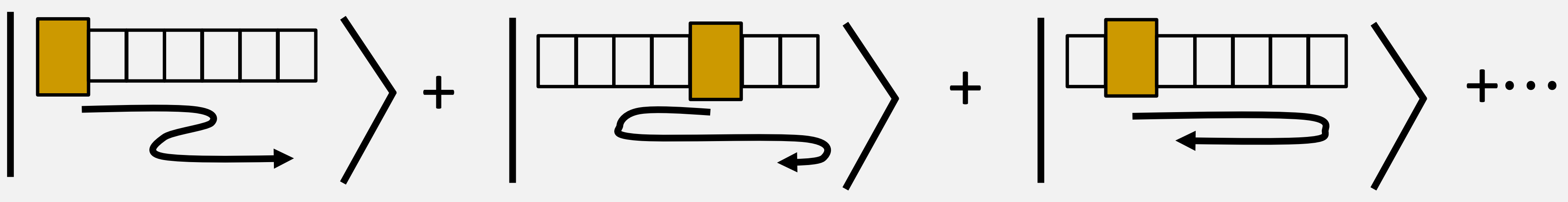




Quantum superposition of dynamics

Until now, we have regarded the state of the system as a single computational basis state.

However, actually, the initial state is a **superposition** of computational basis states, and the dynamics of TMs are also superposition.



Example of superposition of dynamics

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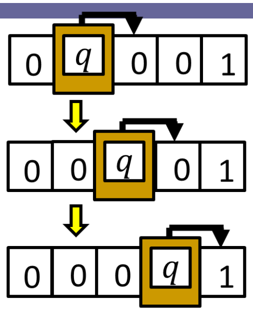
- If TM reads 1, then it stops.



Initial state: $|\psi(0)\rangle = \alpha|0q001\rangle + \beta|0q011\rangle$

$$|0q001\rangle \leftrightarrow |00q01\rangle \leftrightarrow |000q1\rangle$$

$$|0q011\rangle \leftrightarrow |00q11\rangle$$

Time evolution occurs in each gray region separately.

Expanding initial state

The initial state is

$$|\psi_0\rangle \otimes (|\psi_1\rangle)^{\otimes L} = \underline{|\psi_0\rangle} \otimes (\sqrt{\alpha}\,|\text{A-cell}\rangle + \sqrt{1-\alpha}\,|\text{M-cell}\rangle)^{\otimes L}$$

state of TMs

$$|\text{A-cell}\rangle = |a_0\rangle$$

$$|\text{M-cell}\rangle = \underbrace{|0\rangle}_{\text{Layer 1}} \otimes \underbrace{(\sqrt{\beta}\,|1\rangle + \sqrt{1-\beta}\,|0\rangle)}_{\text{Layer 2}} \otimes \underbrace{(\sqrt{\gamma}\,|1\rangle + \sqrt{1-\gamma}\,|0\rangle)}_{\text{Layer 3}}$$

We set $\alpha \simeq 1$ (i.e., **most cells are A-cells**).

Expanding Layer 2

$$(\sqrt{\beta}\,|1\rangle + \sqrt{1-\beta}\,|0\rangle)^{\otimes L}$$

$$= \sum \underbrace{c_{0\cdots00}\,|00\cdots0\rangle + c_{0\cdots01}\,|0\cdots01\rangle + \cdots + c_{1\cdots11}\,|1\cdots11\rangle}_{2^L \text{ states}}$$

Law of large numbers → Almost all states with visible weight have 1 with frequency β.
→ input code **x** is correctly decoded in almost all states!

(Similar argument holds for the type of cells and Layer 3)

Logic flow

In almost all computational basis states in the initial state $|\psi(0)\rangle$, input code **x** is successfully decoded (frequency of 1 is close to β).

⇩

Each computational basis initial state evolves separately, while in all cases its value of A becomes finite iff the URTM with input code **x** halts.

⇩

The initial state $|\psi(0)\rangle$ thermalizes w.r.t. A iff the URTM with input code **x** halts.

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Computational power of thermalization

Our result shows not only undecidability but also **computational universality** of thermalization.

Any computational task can be implemented by thermalization phenomena.

We show a (striking) example.

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

- The presence/absence of thermalization in given systems is **undecidable**.

- This result is still valid for one-dimensional, shift-invariant, nearest-neighbor systems.

- Our result also show that **thermalization can compute any computational task**, which elucidates connection between thermalization and various mathematical tasks.

END

(N. Shiraishi and K. Matsumoto, arXiv:2012.13889/arXiv:2012.13890)