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## Article

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# Undecidability in quantum thermalization

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**The investigation of thermalization in isolated quantum many-body systems has a long history, dating back to the time of developing statistical mechanics. Most quantum many-body systems in nature are considered to thermalize, while some never achieve thermal equilibrium. The central problem is to clarify whether a given system thermalizes, which has been addressed previously, but not resolved. Here, we show that this problem is undecidable. The resulting undecidability even applies when the system is restricted to one-dimensional shift-invariant systems with nearest-neighbour interaction, and the initial state is a fixed product state. We construct a family of Hamiltonians encoding dynamics of a reversible universal Turing machine, where the fate of a relaxation process changes considerably depending on whether the Turing machine halts. Our result indicates that there is no general theorem, algorithm, or systematic procedure determining the presence or absence of thermalization in any given Hamiltonian.**

Thermalization, or relaxation to equilibrium, in isolated quantum many-body systems is a ubiquitous yet profound phenomenon. The history of investigation of thermalization dates back to Boltzmann<sup>1</sup> and von Neumann<sup>2</sup>, and many theoretical physicists have studied this problem. The problem originated in the field of nonequilibrium statistical mechanics. However, some techniques developed in quantum information theory have gained attention to provide fresh insight into this old problem<sup>3</sup>. From the experimental side, the recent development of experimental techniques to manipulate cold atoms enabled us to observe thermalization of isolated quantum many-body systems in the laboratory<sup>4-9</sup>. Experimentalists not only tested established theoretical results, but also revealed some unexpected behaviours<sup>9</sup>.

A central problem in this field is whether a given system thermalizes<sup>3,10</sup>. Although almost all-natural quantum many-body systems are expected to thermalize, some systems, including integrable and localized systems, are known to never achieve thermalization<sup>11-15</sup>. To resolve this problem, the eigenstate thermalization hypothesis (ETH) has been raised as a clue to understanding thermalization phenomena. The ETH claims that all the energy eigenstates of a given Hamiltonian are thermal, that is, indistinguishable from the equilibrium state, as long as we observe macroscopic observables<sup>16-21</sup>. Studies based on numerical simulations support that most non-integrable thermalizing systems satisfy the ETH<sup>20,22-24</sup>. In contrast, recent theoretical studies and elaborated experiments have revealed that some non-integrable thermalizing systems do not satisfy the ETH<sup>9,25-31</sup>. Hence, the ETH does not provide a full characterization of thermalization. Numerous other theoretical ideas, including largeness of effective dimension<sup>10</sup>, typicality<sup>10,32-34</sup>, and quantum correlation<sup>35-37</sup> have been proposed to eluci-

date thermalization phenomena; however, none of them provides a decisive answer.

We approach the problem of thermalization from the opposite side. We examine the difficulty of the problem from the viewpoint of the theoretical computer science. This type of approach is employed in some problems in physics, including prediction of dynamical systems<sup>39</sup>, repeated quantum measurements<sup>40</sup>, and the spectral gap problem<sup>41</sup>. In this approach, these problems were unexpectedly shown to be undecidable, that is, there is no algorithm to determine, e.g., the presence or absence of a spectral gap in arbitrary systems in the case of the spectral gap problem.

Our main achievement in this paper is the finding that whether a given system thermalizes or not is undecidable in general. This result shows not merely the difficulty of this problem, but also the logical impossibility of solving it. Hence, the fate of thermalization in a general setup is independent of the basic axioms of mathematics, as implied in the Gödel's incompleteness theorem<sup>38</sup>. We prove this by demonstrating that thermalization phenomena in one-dimensional systems have the power of universal computation. Our result not only sets a limit on what we can know about quantum thermalization, but also elucidates a rich variety of thermalization phenomena, which can implement any computational task.

## Results

### Statement of main result

We first clarify the precise statement of our result, namely, the undecidability of thermalization. Throughout this study, we consider a one-dimensional lattice system of size  $L$  with the periodic boundary condition (we finally take  $L \rightarrow \infty$  limit), with  $d$ -dimensional local Hilbert space  $\mathcal{H}$ . Let  $|\psi(t)\rangle$  be the state of the

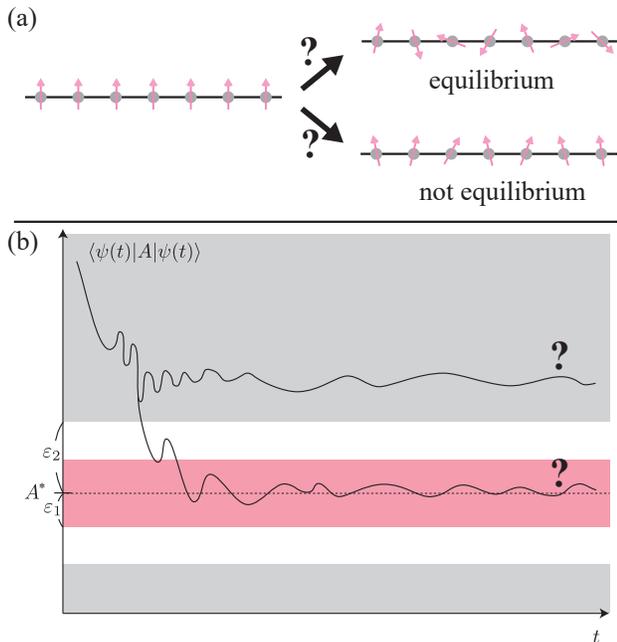


FIG. 1. **The problem of thermalization concerns the long-time average of the observable.**— (a) We consider whether a nonequilibrium initial state relaxes to the equilibrium or not. (b) More precisely, we decide whether the long-time average of  $\langle \psi(t) | A | \psi(t) \rangle$  converges to the value  $A^*$  with precision  $\varepsilon_1$ , or deviates from  $A^*$  at least  $\varepsilon_2 > \varepsilon_1$  (If the long-time average settles between  $\varepsilon_1$  and  $\varepsilon_2$ , we do not have to answer). This problem is shown to be an undecidable problem.

system at time  $t$ . The long-time average of an observable  $A_L$  for a given initial state  $|\psi(0)\rangle = |\psi_0^L\rangle$  is given by  $\bar{A}_L = \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T dt \langle \psi(t) | A_L | \psi(t) \rangle$ . Our interest takes the form of whether the thermodynamic limit of the long-time average  $\bar{A}_L$ , denoted by  $\bar{A} := \lim_{L \rightarrow \infty} \bar{A}_L$ , converges to the vicinity of a given value  $A^*$ . This question concerns the fate of a relaxation process with a given initial state, observable, and Hamiltonian.

We restrict the class of the Hamiltonians, observables, and initial states to simple ones. The Hamiltonian of the system is restricted to be nearest-neighbour interaction and shift-invariant. Hence, the  $d^2 \times d^2$  local Hamiltonian  $h_{i,i+1}$ , which acts only on sites  $i$  and  $i+1$ , fully characterizes the system Hamiltonian as  $H := \sum_i h_{i,i+1}$ . We further restrict observables to a spatial average of a single-site operator:  $A_L := \frac{1}{L} \sum_{i=1}^L A_i$  (for the case of system size  $L$ ), where  $A_i$  acts only on the site  $i$ . We assume that  $A_i$  has at least two distinct eigenvalues. In addition, we restrict the initial state as the following form of a product state:  $|\psi_0^L\rangle = |\phi_0\rangle \otimes |\phi_1\rangle \otimes |\phi_1\rangle \otimes \cdots \otimes |\phi_1\rangle$ , where  $|\phi_0\rangle$  and  $|\phi_1\rangle$  are states on a single site orthogonal to each other;  $\langle \phi_0 | \phi_1 \rangle = 0$ . Even in this very simple setup, we show that whether the long-time average of  $A$  from this initial state  $|\psi_0^L\rangle$  under a given Hamiltonian  $H$

relaxes to the vicinity of a given value  $A^*$  is undecidable.

*Theorem:* Set the dimension of the local Hilbert space  $d$  to be sufficiently large. Given two states  $|\phi_0\rangle$  and  $|\phi_1\rangle$ , orthogonal to each other on a single site, and a single-site operator  $A$  with at least two distinct eigenvalues. Also given are the initial state and the observable as  $|\psi_0^L\rangle = |\phi_0\rangle \otimes |\phi_1\rangle \otimes \cdots \otimes |\phi_1\rangle$  and  $A_L := \frac{1}{L} \sum_{i=1}^L A_i$ . We suppose that there is a promise that either  $|\bar{A} - A^*| < \varepsilon_1$  or  $|\bar{A} - A^*| > \varepsilon_2$  holds with given  $A^*$  and  $0 < \varepsilon_1 < \varepsilon_2$  (see Fig. 1). Then, deciding which is true for a given shift-invariant nearest-neighbour interaction Hamiltonian  $H = \sum_i h_{i,i+1}$  is undecidable.

An alternative expression of the above promise is that we are allowed to output a wrong answer for  $\varepsilon_1 \leq |\bar{A} - A^*| \leq \varepsilon_2$ . If  $A^*$  is equal to the equilibrium value, which can be easily realized, our result reads undecidability of thermalization: Whether a given system with a fixed initial state thermalizes or not with respect to the observable  $A$  is undecidable.

To avoid confusion, we remark that this decision problem is *not* solved by exact diagonalization or any other numerical methods. This decision problem concerns the behaviour in the  $L \rightarrow \infty$  limit, while the exact diagonalization always treats finite-size systems. Any numerical method on finite-size systems cannot exclude the possibility that we overlook the true thermodynamic limit due to the limitation of finite size. This is indeed the case in a family of Hamiltonians that we construct.

### Mapping classical Turing machines to a quantum system

Here, we briefly sketch the main idea of the proof. A rigorous proof is presented in Supplementary material. We first introduce a key ingredient, the halting problem of a Turing machine (TM), which is a prominent example of undecidable problems. The halting problem of a TM asks whether the TM with a given input halts at some time or does not halt and runs forever. Turing proved in his celebrated paper that there exists no general procedure to solve the halting problem<sup>42</sup>.

Following various studies demonstrating undecidability<sup>43</sup>, we first show the following lemma, and then apply the reduction to the halting problem.

*Lemma:* Set the dimension of the local Hilbert space  $d$  to be sufficiently large. Given its complete orthogonal normal sets  $\{|e_i\rangle\}_{i=0}^{d-1}$  and an observable  $A$  satisfying  $\langle e_1 | A | e_1 \rangle = 0$  and  $\langle e_2 | A | e_2 \rangle > 0$  arbitrarily, we fix a universal reversible Turing machine (URTM). Then, for any  $\eta > 0$ , there exists a shift-invariant nearest-neighbor interaction Hamiltonian  $H$  and a set of unitary operators,  $\{V_{\mathbf{x}}\}$ , on the local Hilbert space  $\mathcal{H}$  which satisfies  $V_{\mathbf{x}} |e_0\rangle = |e_0\rangle$  for any  $\mathbf{x}$  and the following property:

Set the initial state as

$$|\psi_0\rangle = (V_{\mathbf{x}} |e_0\rangle) \otimes (V_{\mathbf{x}} |e_1\rangle)^{\otimes L}. \quad (1)$$

If the URTM halts with the input  $\mathbf{x}$ , then

$$\bar{A} \geq \left(\frac{1}{4} - \eta\right) \langle e_2 | A | e_2 \rangle \quad (2)$$

holds, and if the URTM does not halt with the input  $\mathbf{x}$ , then

$$\bar{A} \leq \eta \quad (3)$$

holds.

By adopting the unitary transformation  $V_{\mathbf{x}}^{\otimes L}$  on the Hamiltonian, the degree of freedom in the choice of unitary transformation is mapped to that of the local Hamiltonian. Because the halting problem of the TM is undecidable, the above lemma directly implies the desired theorem and the undecidability of the long-time average in quantum many-body systems. Notably, although the necessary dimension of the local Hilbert space  $d$  is not calculated rigorously, we roughly estimate the sufficient dimension at approximately 100, which is miniscule compared to other results of undecidability in physics<sup>41</sup>.

### Classical machines

Here, we outline the construction of a classical Turing machine, which emulates the halting problem of URTM and changes the long-time average of the observable  $A$  depending on the behaviour of the URTM. This machine emulates three Turing machines, TM1, TM2, and TM3. TM1 decodes the input code  $\mathbf{x}$  for TM2 from a sequence of two qubits. TM2 is a URTM, which runs with the decoded input  $\mathbf{x}$ , whose reversibility is induced by the unique direction property<sup>44</sup>. TM3 is a simple TM, which flips the state of A-cells if and only if TM2 halts. Through the above trick, the long-time average  $\bar{A}$  in our system reflects the result of the halting problem of TM2.

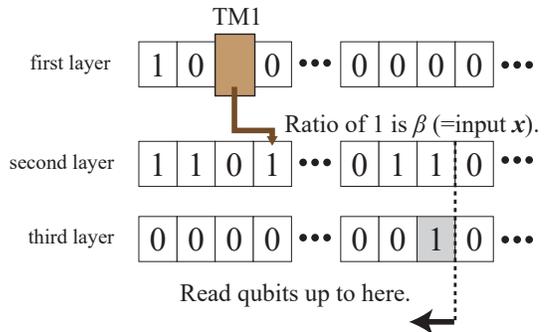
The classical system has two types of cells, M-cells and A-cells. Two Turing machines, TM1 and TM2, are emulated in M-cells. An M-cell consists of three layers: The first layer emulates two Turing machines, and the second and the third layers store the input code of TM2. First, TM1 decodes a bit sequence  $\mathbf{x}$  on the first layer from the second and the third layers (the first part of Fig. 2), and TM2 runs with this input  $\mathbf{x}$ . Throughout this procedure, the machine passes all A-cells transparently.

A-cells are responsible for changing the long-time average of  $A$ . At the initial state, the expectation value of  $A$  in A-cells is set to be zero. If and only if TM2 halts, TM3 starts flipping states of A-cells, and the expectation value of  $A$  becomes a nonzero value. To inflate the difference between the halting and non-halting cases, we set the initial state such that most of the cells are A-cells.

The procedure is summarized as follows:

- (i) TM1 decodes the input code  $\mathbf{x}$  on the first layer.
- (ii) TM2, a URTM, runs with the input  $\mathbf{x}$  in the first layer.

### First part (only M-cells)



### Second part

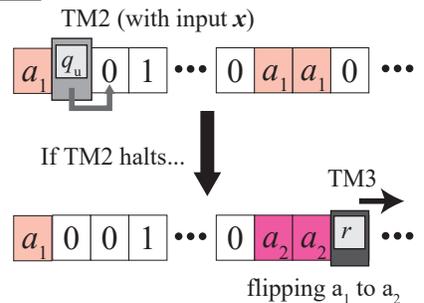


FIG. 2. **Roles of three layers in M-cells and schematic of dynamics of two Turing machines**— [Top]: In the first part, a reversible Turing machine, TM1, decodes a bit sequence  $\mathbf{x}$  on the first layer through the estimation of the number of  $|1\rangle$  in the second layer (step (i)). The binary expansion of  $\beta$  is set to  $\mathbf{x}$ . The number of qubits TM1 reads is determined by the leftmost cell with 1 in the third layer. Here, we draw only M-cells and omit A-cells for visibility. [Bottom]: In the second part, a universal reversible Turing machine, TM2, runs with the input  $\mathbf{x}$  (step (ii)). If TM2 halts, then TM3 starts to flip the state in the second layer from  $a_1$  to  $a_2$  (step (iii)). If TM2 does not halt, the sites in the second layer are not flipped. Note that we have not drawn the second and third layers of M-cells for visibility.

- (iii) If and only if TM2 halts, then TM3 starts flipping the states in A-cells (see the second part of Fig. 2). This induces a visible difference between the long-time average of  $A$  in the case of halting and non-halting.
- (iv) In case of halting, the head returns to the cell, where TM2 halts due to the periodic boundary condition. By this time, all A-cells have already been flipped, and TM3 stops.

Because the halting problem of TM2 with an arbitrary input  $\mathbf{x}$  is undecidable, the long-time average of  $A$  with an arbitrary local unitary transformation  $V_{\mathbf{x}}$  is likewise undecidable.

### Hamiltonian construction and its eigenstates

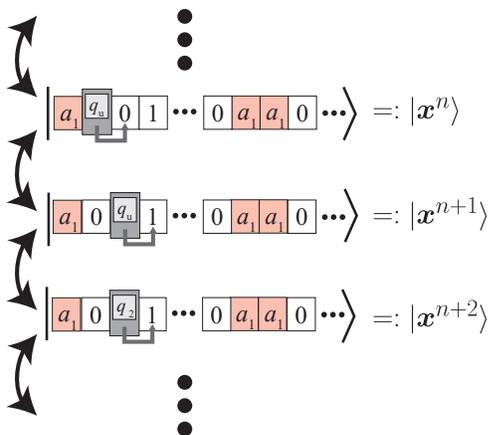


FIG. 3. **Evolution of the quantum state of the total system**— We draw a possible hopping between quantum states in the computational basis. Although here, we depict only the first and second layers for visibility, the quantum state actually consists of three layers. Similar to the Feynman-Kitaev Hamiltonian case, the total Hamiltonian induces the forward and backward one-step time evolution of the TM.

Our implementation of the classical TM in quantum systems stems from the construction of the Feynman-Kitaev Hamiltonian<sup>45,46</sup>, while we delete the clock part. Each site takes one of the states of the finite control or that of a single cell in the tape, or some additional symbols. If the site  $i$  is a state of the finite control, then the head reads the site  $i+1$  or  $i-1$  (see Fig. 3). In the initial state, we set the finite control at site 1, and set all other sites not to the states of the finite control. Because the dynamics conserve the number of sites of the finite control, only a single site takes the state of the finite control at all times.

The dynamics of TM are encoded in the local Hamiltonian as follows. Suppose, e.g., that the cell at the head is  $s_a$ , the state of the finite control is  $q_b$ , and the URTM (TM2) moves to the right. Then, the local Hamiltonian  $h_{i,i+1}$  must contain the term

$$|s_a, q_b\rangle \langle q_b, s_a| + \text{c.c.} \quad (4)$$

In a similar manner, we add all transition rules of TMs (both TM1, TM2, and TM3) to the local Hamiltonian in the form of (4). Owing to the deterministic property of TMs, all the legal states of the total system have a unique descendant state.

Because the decoding process is slightly complicated, we first take an analogous and easier setting and present the basic idea of construction. Our original setting is discussed in the following section. We set the initial state as a non-uniform computational basis state, such that decoding of the input code  $\mathbf{x}$  has no quantum fluctuation. Let  $|\mathbf{x}^1\rangle$  denote the initial configuration of the total system, and  $|\mathbf{x}^n\rangle$  be the  $n$ -th state (i.e., after  $n-1$  steps from  $|\mathbf{x}^1\rangle$ ). By restricting the Hilbert space to the subspace

spanned by  $\{|\mathbf{x}^n\rangle\}$ , the total Hamiltonian is expressed as (see also Fig. 3)

$$H' = \sum_{n=1}^{J-1} |\mathbf{x}^{n+1}\rangle \langle \mathbf{x}^n| + \text{c.c.}, \quad (5)$$

where the  $J$ -th state is the final state of this dynamics. This Hamiltonian takes the same form as a single-particle system on a closed one-dimensional lattice with only the hopping term. Employing the result on a tridiagonal matrix, eigenenergies and energy eigenstates are calculated as

$$E_j = 2 \cos\left(\frac{j\pi}{J+1}\right) \quad (6)$$

$$|E_j\rangle = \sqrt{\frac{2}{J+1}} \sum_{k=1}^J \sin\left(\frac{kj\pi}{J+2}\right) |\mathbf{x}^k\rangle \quad (7)$$

with  $j = 1, 2, \dots, J$ .

By expanding the initial state as  $|\mathbf{x}^1\rangle = \sum_{j=1}^J c_j |E_j\rangle$ , the long-time average of  $A$  reads  $\bar{A}_L = \sum_{j=1}^J |c_j|^2 \langle E_j | A | E_j \rangle$ , because all the off-diagonal elements vanish in the long-time average. Since the number of steps until TM2 halts is independent of the system size  $L$ , by setting  $L$  to be sufficiently large, we can make the flipping of A-cells start before  $J/2$  steps. In this condition, half of the A-cells have been flipped before  $3J/4$  steps, which confirms the nonzero expectation value of  $\bar{A}_L$  in the case of halting. In contrast, in the case of non-halting, the flipping by TM3 does not occur, and hence the long-time average  $\bar{A}_L$  is kept close to zero.

### Uniform initial state

We now describe the decoding process from the second and third layers of M-cells in our original setting. The second and third layers are set to  $\sqrt{\beta}|1\rangle + \sqrt{1-\beta}|0\rangle$  and  $\sqrt{\gamma}|1\rangle + \sqrt{1-\gamma}|0\rangle$ , respectively. The state on  $m$  of M-cells is a superposition of  $2^m \times 2^m$  computational basis states. TM1 runs on each computational basis state, and thus the dynamics of TMs is also a superposition of  $2^m \times 2^m$  branches.

The quantity  $\beta$  stores the input code in the form such that the binary expansion of  $\beta$  equals the input code  $\mathbf{x}$ . TM1 calculates  $\beta$  by estimating the relative frequency of the state  $|1\rangle$  in the second layer. Due to the law of large numbers, the set of computational basis states, where the relative frequency of  $|1\rangle$  is close to  $\beta$ , has an arbitrarily large probability amplitude. The quantity  $\gamma$  (more precisely,  $-1/\ln \gamma$ ) characterizes the length of qubits that TM1 must read in. TM1 reads the qubits in the second layer until it first encounters  $|1\rangle$  in the third layer (the first part of Fig. 2). By setting  $\gamma$  to be sufficiently small, the probability of two unwanted cases, namely, (a) TM1 stops decoding before  $\mathbf{x}$  is decoded to the last, and (b) TM1 can access only an insufficiently small number of qubits in the second layer and fails to estimate the correct  $\beta$ , becomes negligible.

## Discussion

The presence or absence of thermalization in a given quantum many-body systems, which has been a topic of debate among researchers in various fields, is proven to be undecidable. Hence, there exists no general systematic procedure to determine the long-time behaviour of quantum many-body systems. The undecidability is still valid for a class of simple systems; one-dimensional systems with a shift-invariant and nearest-neighbour interaction. Our result leads to a fundamental limitation to reach a general theory on thermalization. This finding implies that analyses based on a concrete model or a restricted class of systems might be more fruitful to facilitate our theoretical and rigorous understanding of thermalization phenomena.

Our proof also shows the computational universality of thermalization phenomena. Contrary to apparent simplicity of thermalization phenomena, the above fact leads to an astonishing consequence that the variety of thermalization phenomena is at the same level as that of tasks computers can treat. A striking example bridging physics and mathematics is a system which thermalizes if and only if the Riemann hypothesis is true. The above system reflects the existence of a TM which halts if and only if the Riemann hypothesis is false<sup>47</sup>.

From a physical context, extremely slow relaxation of our model in case of halting is induced by quasi-conserved quantities, which are close to conserved quantities but not conserved. Recently, some non-integrable systems (the transverse Ising model with  $z$  magnetic field) have been reported to relax very slowly, which is also caused by quasi-conserved quantities<sup>23,48,49</sup>. Numerical simulations with ordinal size and time length fail to address thermalization in these systems. The extremely slow relaxation in our system might be understood from the aforementioned more general viewpoint, which is worth further investigation.

We finally comment on the limitations of our result and conclude this study. First, our result does not exclude the possibility that one proves the presence or absence of thermalization in specific systems. Our result only excludes the possibility to obtain a general and ultimate criterion to judge the presence or absence of thermalization. In fact, integrable systems are known not to thermalize. Second, our undecidability is shown in only a highly artificial model with a particular form of Hamiltonians, which is another limitation of our result. One needs to proceed to a more *natural* model exhibiting undecidability, or to find a set of a restricted class of physical Hamiltonians whose fate of thermalization is now decidable. These problems are left for future investigations.

## Method

### Expression of long-time average

We here show a general expression of the long-time average

$\bar{A}$ . Let  $H$  be a Hamiltonian of the system, and  $E_i$  and  $|E_i\rangle$  be eigenenergy and corresponding energy eigenstate. An initial state  $|\psi\rangle = \sum_i c_i |E_i\rangle$  evolves under the Hamiltonian  $H$ . Then, the long-time average of an observable  $A$  is calculated as

$$\begin{aligned}\bar{A} &= \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T dt \langle \psi(t) | A | \psi(t) \rangle \\ &= \lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T dt \sum_{i,j} e^{-i(E_j - E_i)t} \langle E_i | A | E_j \rangle \\ &= \sum_{i,j} \chi(E_j = E_i) \langle E_i | A | E_j \rangle,\end{aligned}\quad (8)$$

where  $\chi(E_j = E_i)$  takes 1 if  $E_j = E_i$  and takes zero otherwise. We set the Planck constant to unity. In the third line, we used the fact that  $\lim_{T \rightarrow \infty} \frac{1}{T} \int_0^T dt e^{-i(E_j - E_i)t}$  converges to zero if  $E_j \neq E_i$  and equal to 1 if  $E_j = E_i$ . If the Hamiltonian  $H$  has no degeneracy, we have a concise expression  $\bar{A} = \sum_i \langle E_i | A | E_i \rangle$ . In contrast, if there exist degeneracy ( $E_i = E_j$  with  $i \neq j$ ), we need to handle off-diagonal elements  $\langle E_i | A | E_j \rangle$ .

### Decoding from the second and third layers

We discuss how to decode the input code  $\mathbf{x}$  from the sequence of two qubits in the second and third layers. The amount of  $\beta$ , whose binary expansion is equal to  $\mathbf{x}$ , is guessed by the relative frequency of 1's in the second layer (see Fig. 2). We expand  $m$  copies of  $\sqrt{\beta}|1\rangle + \sqrt{1-\beta}|0\rangle$  as

$$\begin{aligned} & (\sqrt{\beta}|1\rangle + \sqrt{1-\beta}|0\rangle)^{\otimes m} \\ &= \sum_{\mathbf{w} \in \{0,1\}^{\otimes m}} \sqrt{\beta}^{N_1(\mathbf{w})} \sqrt{1-\beta}^{m-N_1(\mathbf{w})} |\mathbf{w}\rangle,\end{aligned}\quad (9)$$

where  $\mathbf{w}$  is a sequence of 01 with length  $m$ , and  $N_1(\mathbf{w})$  is the number of 1's in the binary sequence  $\mathbf{w}$ . The probability amplitude for a state  $|\mathbf{w}\rangle$  is  $|c_{\mathbf{w}}|^2 = \beta^{N_1(\mathbf{w})} (1-\beta)^{m-N_1(\mathbf{w})}$ . Due to the law of large numbers, the probability amplitude for states with relative frequency of 1's close to  $\beta$  converges to 1 in the large  $m$  limit:

$$\lim_{m \rightarrow \infty} \sum_{\mathbf{w}: \frac{N_1(\mathbf{w})}{m} \simeq \beta} |c_{\mathbf{w}}|^2 = 1. \quad (10)$$

Here, the symbol  $\frac{N_1(\mathbf{w})}{m} \simeq \beta$  means that  $\frac{N_1(\mathbf{w})}{m}$  is close to  $\beta$ , whose rigorous definition is presented soon later (in Eq. (12)). Hence, if  $m$  is sufficiently large compared with the length of the input code, TM1 guesses  $\beta$  correctly from the frequency of 1's.

The length  $m$  is determined by another bit sequence,  $\sqrt{\gamma}|1\rangle + \sqrt{1-\gamma}|0\rangle$ , in the third layer. Let  $0 < \xi < 1$  be a given accuracy. We encode the information of  $m$  into  $\gamma$  as satisfying

$$(1-\gamma)^m \geq 1-\xi. \quad (11)$$

In other words, almost all qubits are  $|0\rangle$  in this sequence, and  $|1\rangle$  appears only after  $m$ -th digit with probability larger than  $1-\xi$ . Owing to this, if  $|1\rangle$  appears at the  $m'$ -th digit for the first time, this is taken as the sign that  $m \leq m'$ . Based on the observed value  $m'$ , the length of the output by TM1 (i.e., the presumed length of the digit of  $\beta$ ) is determined as  $n' = \lceil \frac{1}{4} \log_2 m \rceil$ , which ensures

$$\lim_{m \rightarrow \infty} \text{Prob} \left[ \left| \frac{N_1(\mathbf{w})}{m} - \beta \right| < \frac{1}{2^{n'+1}} \right] = 1. \quad (12)$$

With the choice of this output length  $n'$ , guessing  $m$  larger than the true value does not affect the correctness of the estimation of  $\beta$ .

## Proofs

All the results in this paper are rigorously proved in the Supplementary material.

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### Author contributions

NS and KM contributed equally to this work.

### Competing Interest

The authors declare no competing interest.

# Figures

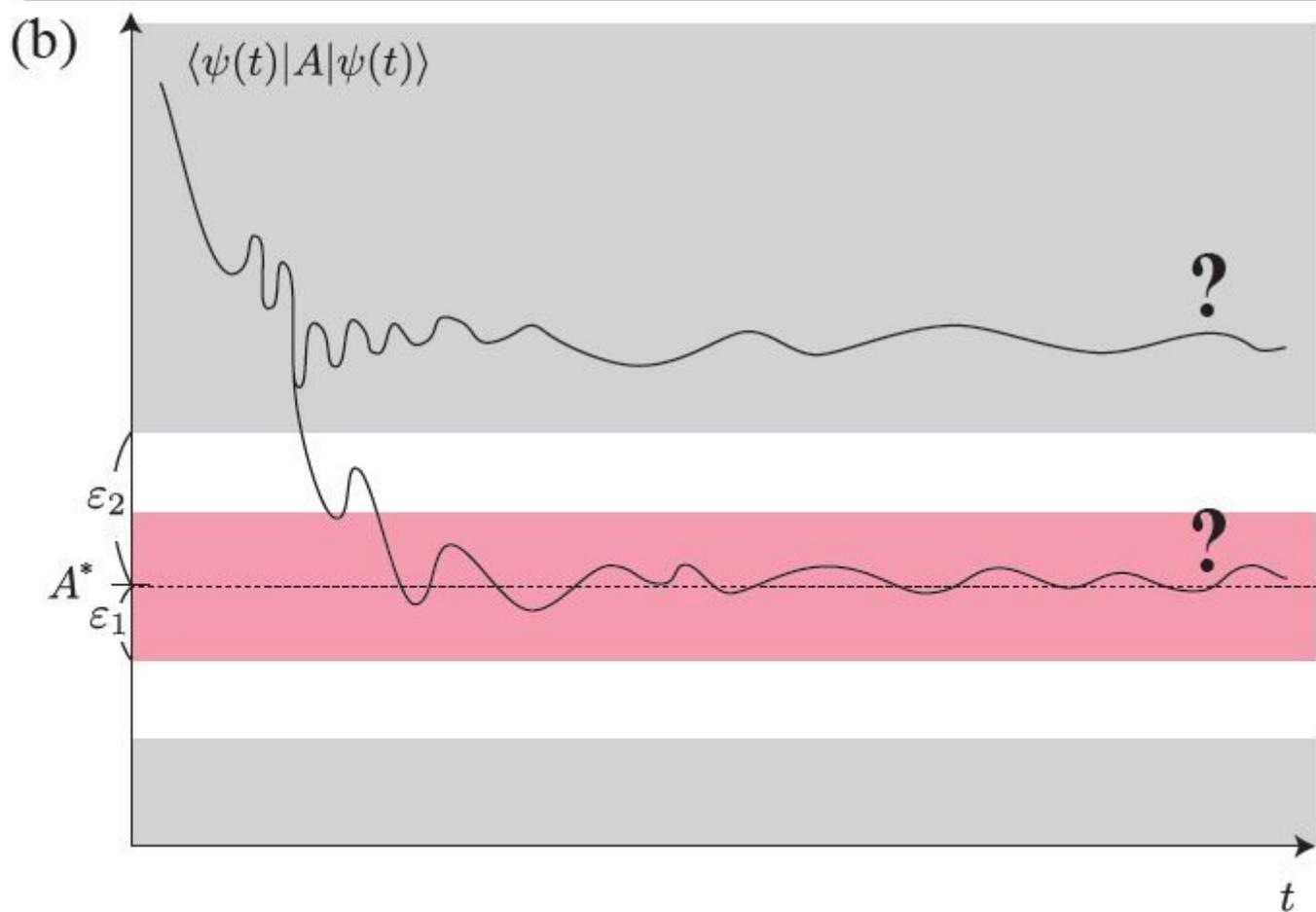
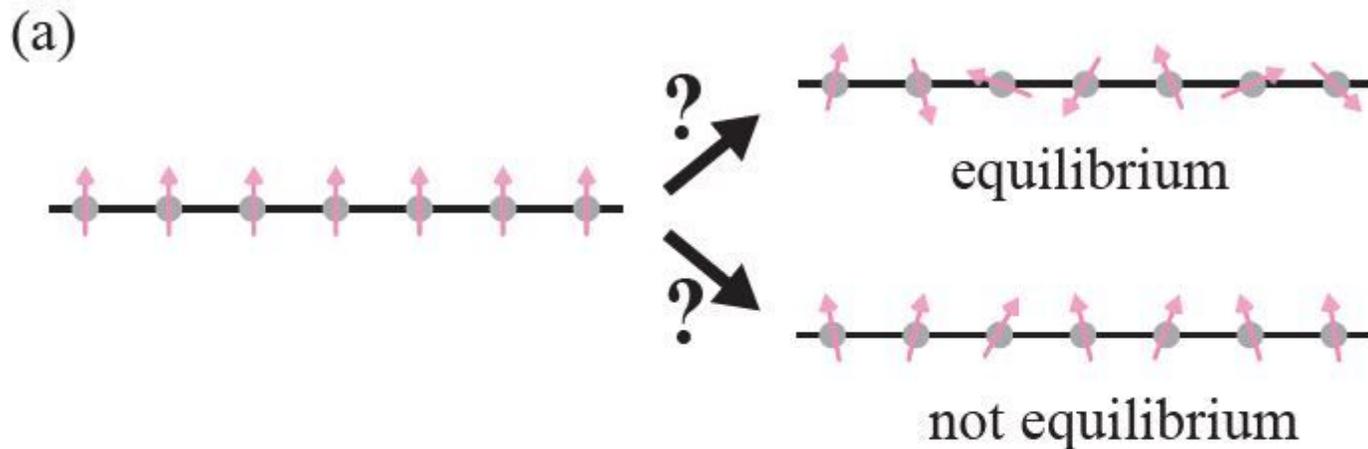
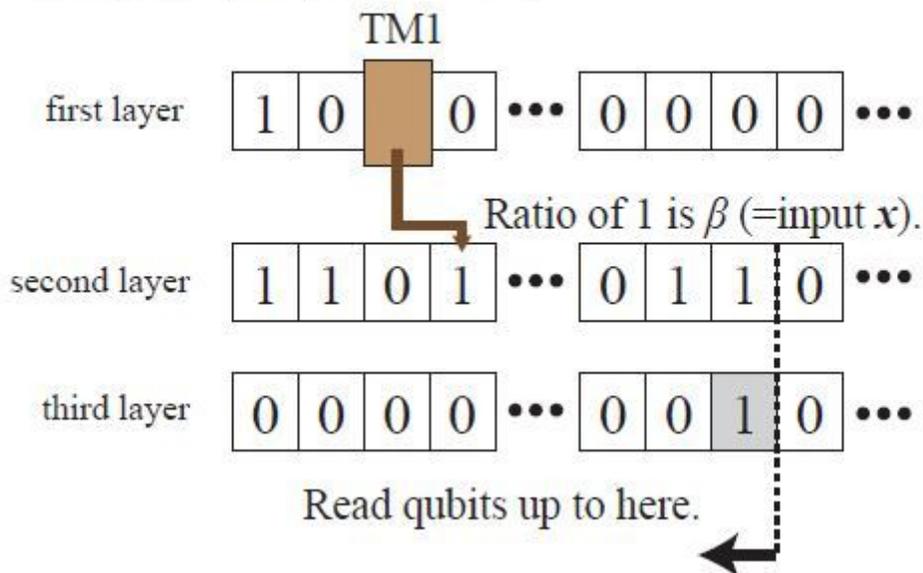


Figure 1

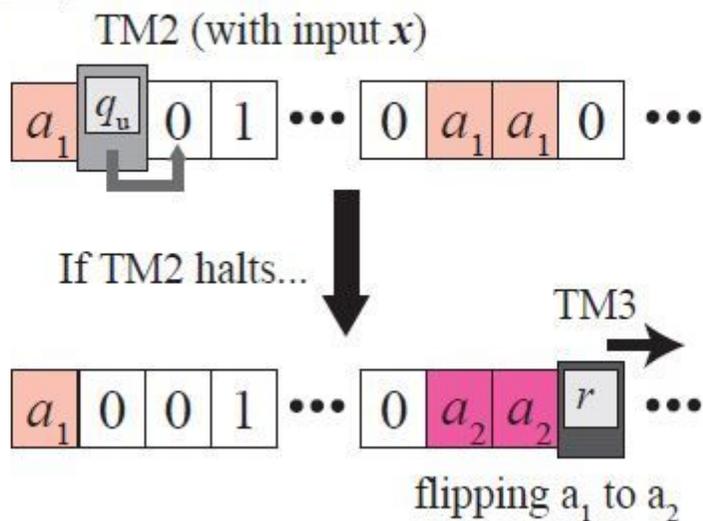
The problem of thermalization concerns the long-time average of the observable.— (a) We consider whether a nonequilibrium initial state relaxes to the equilibrium or not. (b) More precisely, we decide whether the long-time average of  $\langle \psi(t) | A | \psi(t) \rangle$  converges to the value  $A^*$  with precision  $\epsilon_1$ , or deviates from

$A$  at least  $\epsilon_2 > \epsilon_1$  (If the long-time average settles between  $\epsilon_1$  and  $\epsilon_2$ , we do not have to answer). This problem is shown to be an undecidable problem.

### First part (only M-cells)



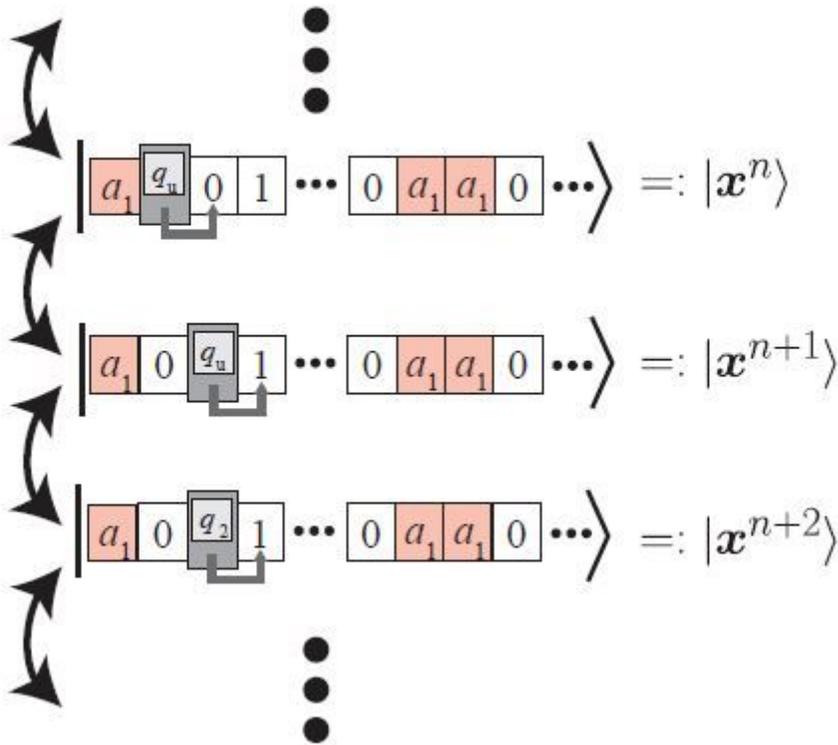
### Second part



**Figure 2**

Roles of three layers in M-cells and schematic of dynamics of two Turing machines— [Top]: In the first part, a reversible Turing machine, TM1, decodes a bit sequence  $x$  on the first layer through the estimation of the number of 1 in the second layer (step (i)). The binary expansion of  $\beta$  is set to  $x$ . The number of qubits TM1 reads is determined by the leftmost cell with 1 in the third layer. Here, we draw only M-cells and omit A-cells for visibility. [Bottom]: In the second part, a universal reversible Turing machine, TM2, runs with the input  $x$  (step (ii)). If TM2 halts, then TM3 starts to flip the state in the second layer from  $a_1$

to  $a_2$  (step (iii)). If TM2 does not halt, the sites in the second layer are not flipped. Note that we have not drawn the second and third layers of M-cells for visibility.



**Figure 3**

Evolution of the quantum state of the total system— We draw a possible hopping between quantum states in the computational basis. Although here, we depict only the first and second layers for visibility, the quantum state actually consists of three layers. Similar to the Feynman-Kitaev Hamiltonian case, the total Hamiltonian induces the forward and backward one-step time evolution of the TM.

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