Analytic model of thermalization: Quantum emulation of classical cellular automata

Naoto Shiraishi

Department of physics, Keio university, Hiyoshi 3-14-1, Kohoku-ku, Yokohama, Japan
(Dated: July 3, 2018)

We introduce a novel method of quantum emulation of a classical reversible cellular automaton. By applying this method to a chaotic cellular automaton, the obtained quantum many-body system thermalizes while all the energy eigenstates and eigenvalues are solvable. These explicit solutions allow us to verify the validity of some scenarios of thermalization to this system. We find that two leading scenarios, the eigenstate thermalization hypothesis scenario and the large effective dimension scenario, do not explain thermalization in this model.

I. INTRODUCTION

Presence and absence of thermalization in quantum many-body systems is one of the most profound problems in theoretical physics. In a broad class of quantum systems, a nonequilibrium initial state relaxes to the unique equilibrium state \([1, 2]\). This phenomenon is called thermalization. However, provably, some quantum systems including integrable systems and localized systems do not show thermalization \([3, 4]\). Thus what determines the presence or absence of thermalization and why thermalization occurs has been intensively studied.

There are mainly two approaches to tackle this problem. One approach employs numerical simulations, which has discovered many interesting phenomena and properties in nonequilibrium relaxation dynamics \([4, 7–12]\). However, it is not easy to establish a theoretical framework from numerical data. In addition, numerical simulations inevitably face the limitation of finite size and finite time, which has sometimes led to incorrect expectations \([12, 13]\). The other approach investigates mathematical foundations, where many general theorems have been proven rigorously \([14–23]\). Nevertheless, most studies concern properties irrelevant to (non)integrability and fail to address the difference between integrable and non-integrable systems, since it is very difficult to prove general theorems clarifying this difference. To break this impasse, we propose another approach; constructing elaborated models which thermalize but can be treated analytically in some sense. In many research fields, artificial but elaborated analytically-accessible models, which support or disprove some conjectures in theoretical physics, are employed. One example is quantum integrable systems which support or disprove some conjectures in theoretical physics. In a broad class of quantum systems, a nonequilibrium initial state relaxes to the unique equilibrium state \([1, 2]\).

In this paper, we propose a novel type of quantum model which emulates (quantizes) a classical cellular automaton (CA). This model is shift-invariant, has local interaction, and its local Hilbert space is small. These properties are conventionally required for physical many-body systems. The emulation can be performed for both integrable and chaotic CA. The advantage of this model lies in the fact that all the energy eigenstates and eigenenergies are solvable even in case of a chaotic CA. Using the expression of energy eigenstates, we verify two leading scenarios of thermalization \([3, 4]\) analytically. Maybe surprisingly, although this model thermalizes, this model neither satisfy the above two scenarios.

This paper is organized as follows. Before discussing quantum systems, in Sec. I we briefly explain the classical second-order reversible CA. In Sec. II we construct the quantum model emulating the classical second-order reversible CA. Notably, all the energy eigenstates and eigenenergies of this quantum model are formally solvable regardless of whether the emulated classical CA is integrable or chaotic. This fact is demonstrated in Sec. IV. With the help of this formal solution, in Sec. V we analytically show that this quantum model thermalizes but this thermalization is not explained by two leading scenarios of thermalization. In Sec. VI, we generalize this model in order to recover the extensivity with keeping analytic properties.
evolution, which we call cycle (see Fig. 1). We label a cycle as \( k \) \((1 \leq k \leq K)\), where \( K \) is the number of all possible cycles. We denote the length of a cycle \( k \) by \( u_k \), which satisfies \( \sum_k u_k = d^{2L} \). For each cycle \( k \), we fix a state as the initial state \( x^0_k \), and write the state of the site \( i \) at the \( n \)-th step as \( x^i_{k,n} \).

We here summarize some known properties of reversible CA with \( d = 2 \). Takesue [38, 39] has reported its thermodynamic properties. Some CA (e.g., 90R) have local conserved quantities, which can be regarded as a counterpart of integrable systems. Some CA (e.g., 73R) have localized states, i.e., if a certain local structure appears in the initial state, this structure never disappears. Other CA (e.g., 214R) neither have local conserved quantities nor localized states, and some of them show chaotic behavior in numerical simulations. An example is seen in Ref. [37], where the CA with the rule 214R appears to thermalize. Throughout this letter we use the word chaotic CA in a loose sense that the CA thermalizes (see also Appendix A).

The length of the cycles has also been numerically investigated [38, 39]. In some CA the maximum and averaged length of cycles is exponentially large \((u \sim 2^L)\). However, in any case its proportion to the size of the state space is exponentially small \((u/d^{2L} \sim 2^{-L})\). We note that in any rule there exists a cycle with very short length, which stems from the fact that any CA keeps spatial periodicity [40].

It is worth comparing the chaotic CA and the chaotic classical billiard system. Similar to the chaotic billiard system, the chaotic CA has many periodic orbits. In contrast, differently from the chaotic billiard system, the chaotic CA shows the mixing property only locally, not globally. This difference is considered to come from the difference between few-body chaos and many-body chaos.

### III. Quantum Emulation of Classical CA

We now introduce a quantum system which emulates a second-order classical reversible CA. Consider a three-layered one-dimensional quantum system with length \( L \), where the top row is head system and the bottom two rows are CA system. The head system consists of a single free fermion, which controls the dynamics of the CA system. The CA system consists of \( 2L \) spins with \( d \) degrees of freedom, which emulates a given classical CA.

Let \( a_{i,1} \) and \( a_{i,2} \) be the states of the \( i \)-th site in the first and second layer of the CA system, and \( c_i \) and \( c_i^\dagger \) be the annihilation and creation operator of the head fermion at the \( i \)-th site. By denoting the product state of the CA system at sites \( i \) and \( i \pm 1 \) as

\[
|a_{i-1}, a_i, a_{i+1}, c_i, c_{i+1}^\dagger\rangle_i
\]

### II. Second-Order Reversible Cellular Automata

Before constructing the model, we briefly review reversible classical CA. We first explain a standard one-dimensional CA, which is not reversible in general, with length \( L \) and the periodic boundary condition. Suppose that each site takes \( d \) possible states in \( S_d := \{0, 1, \ldots, d - 1\} \). For simplicity, we consider the case that the state of the site \( i \) at the next step only depends on the present states of sites \( i \) and \( i \pm 1 \). By denoting \( x^i_n \) the state of the site \( i \) at the \( n \)-th step, the rule of a CA is expressed as \( x^i_{n+1} = f(x^i_{n-1}, x^i_n, x^i_{n+1}) \). Here, \( f \) is a map of \((S_d)^3 \rightarrow S_d \) and thus there are \( d^{3L} \) possible rules. In particular, the CA with \( d = 2 \) has 256 rules, which are labeled from 0 to 255 by Wolfram code [37]. The explicit definition and an example of Wolfram code is presented in Appendix B.

Using the map \( f \), we construct a kind of reversible CA named second-order reversible CA as

\[
x^i_{n+1} \equiv f(x^i_{n-1}, x^i_n, x^i_{n+1}) - x^i_{n-1} \mod d. \tag{1}
\]

It is easy to check that if a trajectory of time evolution \( \cdots \rightarrow x^{n-1} \rightarrow x^n \rightarrow x^{n+1} \cdots \) can realize under a rule, then its time reversal \( \cdots \rightarrow x^{n+1} \rightarrow x^n \rightarrow x^{n-1} \cdots \) can also realize under the same rule. By regarding the pair of a present state \( x^n \) and its last-minute state \( x^{n-1} \) as a (generalized) state, the time evolution \((x^{n-1}, x^n) \rightarrow (x^n, x^{n+1})\) becomes a one-to-one map of states. In this picture, the state space has \( d^{2L} \) possible states. The rules of such reversible CA with \( d = 2 \) are labeled by adding R to the corresponding Wolfram code such as 214R. Because the number of possible states is finite, the state space is decomposed into some cyclic trajectories of time-
This model

Conventional free fermion

The total Hamiltonian of the system is given by $H = \sum_{i=1}^{L} h_i$. Owing to the boundary condition, a single circle move of the fermion $1 \rightarrow 2 \rightarrow \cdots \rightarrow L \rightarrow 1$ induces one-step time evolution of the CA.

The structure of the solution is close to that of a free fermion system and that of this model. Although the structure of these two is similar, the length of the cyclic path of this model is elongated from $L$ to $u_k L$. The factor $u_k$ might increase exponentially with respect to $L$.

IV. EXACT ENERGY EIGENSTATES AND EIGENVALUES

A remarkable point of this model is that all the energy eigenstates and eigenvalues can be explicitly written down with the help of the knowledge of the emulated classical CA. We introduce a basis of the CA system written as

$$|X_{k,i}^n\rangle := \left| \begin{array}{cccc} x_{k,1}^n & \cdots & x_{k,1}^{n-1} & x_{k,L}^{n-1} \\ x_{k,1}^{n+1} & \cdots & x_{k,1}^{n} & x_{k,L}^{n-1} \\ \vdots & & \vdots & \vdots \\ x_{k,1}^n & \cdots & x_{k,1}^{n-1} & x_{k,L}^{n-1} \end{array} \right\rangle$$

with $1 \leq n \leq u_k$, $1 \leq i \leq L$, and $1 \leq k \leq K$, which we also call computational basis. Using this, all the energy eigenstates and corresponding eigenenergies are expressed as

$$E_{k,m} = \frac{1}{\sqrt{u_k L}} \sum_{n=1}^{u_k} \sum_{i=1}^{L} e^{-\frac{2\pi i m (n - \frac{L+1}{2})}{u_k L}} |X_{k,i}^n\rangle \otimes |i\rangle$$

with $m = 0, 1, \cdots, u_k L - 1$. Here, $|i\rangle$ represents the state of the head system that the fermion is at the site $i$. The form of the energy eigenstate directly follows from a simple but crucial relation

$$H(|X_{k,i}^n\rangle \otimes |i\rangle) = |X_{k,i+1}^n\rangle \otimes |i+1\rangle + |X_{k,i-1}^n\rangle \otimes |i-1\rangle$$

The structure of the solution is close to that of a free fermion, while the length in the state space is elongated from $L$ to $u_k L$ (see Fig. 3). We note that some CA has $u_k = O(e^L)$. 

![Diagram](image-url)
V. ANALYTIC RESULTS ON QUANTUM THERMALIZATION

Our calculation on the quantum model before here does not rely on properties of emulated CA. To investigate thermalization phenomena by using this model, we now focus on chaotic CA. Although we do not specify the concrete rule, on the basis of the numerical observations \textit{[37,39]}, it is highly plausible that some CA with some \(d\) is indeed a chaotic CA. In the track of quantization of few-body billiard systems, we assume the existence of a second-order reversible chaotic CA, which satisfies the following three properties in the thermodynamic limit (The precise statements are shown in Appendix C):

(i) \textit{Thermalization}: If we observe only a local region \(C_{i,l}\) with fixed \(l\), then time evolution from an initial state with no spatial periodicity provides the uniform distribution of possible \(d^2\) states.

(ii) \textit{Many cycles}: The maximum length of a cycle is exponentially small compared to the number of possible states; \(d^2 L\).

(iii) \textit{No coherence}: If we observe a region \(C_{i+1,l}\) with fixed \(l\), then almost all states appear at most once in a fixed cycle.

We here denote by \(C_{i_1,i_2}\) \((i_1 < i_2)\) a subsystem of the CA system with sites \(i_1 \leq i \leq i_2\). (If \(i_2 > L\), then \(C_{i_1,i_2}\) represents the subsystem with sites \(i_1 \leq i \leq L\) and \(1 \leq i \leq i_2 - L\)). The counterparts of the conditions (i) and (ii) in a chaotic billiard system are the mixing property and the fact that there are exponentially many periodic orbits. The condition (iii) is strongly suggested by the condition (ii) for the following surmise: The number of states which share states of all sites except \(C_{1,l}\) is only \(d^2 = O(1)\), while a single cycle covers exponentially small proportion of the exponentially large state space. Thus, it is highly plausible to consider that such a short cycle passes a set of states with the size \(O(1)\) at most once.

We fix a chaotic CA which satisfies the aforementioned conditions. Then, in terms of macroscopic observables of the CA system, all the energy eigenstates without spatial periodicity are thermal. This fact is guaranteed by the condition (i) and (iii): The condition (i) ensures the equipartition in view of the computational basis, and the condition (iii) ensures the absence of coherence. Since we cannot prepare a truly spatially-periodic state in a macroscopic system at finite temperature, we confirm that the CA system thermalizes after a physical quench [11].

Owing to the exact solutions, we draw many analytic results on this model. We in particular verify the validity of two leading scenarios of thermalization, the eigenstate thermalization hypothesis (ETH) scenario and the large effective dimension scenario [30], in this model. The first scenario relies on the ETH, which claims that all the energy eigenstates are thermal [3, 14, 15, 42, 44]. The ETH is known to be a sufficient condition for thermalization [21, 36]. Numerical simulations show that the ETH is indeed satisfied in many non-integrable models [3, 7, 9], and thus the ETH is believed to be satisfied in chaotic thermalizing systems. Contrary to this, the ETH with respect to macroscopic observables in the CA system is not satisfied in our model. The violation of the ETH stems from the fact that spatially periodic states have very short period as explained and the corresponding energy eigenstates are not thermal. This model is another counterexample to the ETH different from Refs. [45, 46]. We remark that the violation of the ETH is inherent to the emulation of a CA and it does not rely on the assumptions (i)-(iii).

The second scenario of thermalization is the large effective dimension scenario [17, 36, 37], which claims that an initial state not concentrated on small number of energy eigenstates thermalizes. The effective dimension \(D_{\text{eff}}\) of a pure state |\(\psi\rangle\) is defined as

\[
D_{\text{eff}} := \left( \sum_n |\langle E_n |\psi\rangle|^4 \right)^{-1},
\]

where |\(E_n\rangle\) is the \(n\)-th energy eigenstate. The effective dimension takes \(1 \leq D_{\text{eff}} \leq D\) with the dimension of the Hilbert space of the energy shell \(D\), and it quantifies how many energy eigenstates the state |\(\psi\rangle\) effectively covers. It has been proven that if the effective dimension of an initial state is not exponentially small compared to \(D\) (i.e., \(D_{\text{eff}} / D = \text{poly}(1/L)\)), then this initial state thermalizes [35, 48]. The precise statement of this theorem is shown in Appendix D. Numerical simulations on some specific models support the large effective dimension scenario [10, 11]. In our model, the effective dimension of some initial states can be calculated explicitly. Let us take an initial state |\(\psi_{\text{ini}}\rangle\) such that the head system is |\(i\rangle\) for some \(i\) and the CA system is one of the computational basis vectors. Then, the effective dimension of |\(\psi_{\text{ini}}\rangle\) is exactly same as the length of the cycle to which the state belongs, and the condition (ii) says that it is exponentially small compared to the dimension; \(D = (2d)^L\). It is hence concluded that thermalization in a sector with the aforementioned initial state is not explained by the large effective dimension scenario.

VI. GENERALIZATION TO MANY HEAD PARTICLES

A. Model construction

The presented model has only a single fermion in the head system and thus \(L \to \infty\) limit is not the conventional thermodynamic limit. To realize the conventional thermodynamic limit, we generalize our model to many fermions (or hard-core bosons) with a little modified assumptions on CA.
Replace the head system from a single fermion to $N$ interacting fermions (or hard-core bosons) whose hopping still couples to update of the CA system. We suppose that these particles jump only to its neighboring sites. The Hamiltonian with length $L$ and $N$ particles is then constructed as

$$H = \sum_{i=1}^{L} h_i + V(n)$$

where we defined $n := \{n_1, n_2, \ldots, n_L\}$, and $n_i := c_i^\dagger c_i$ is the number operator at the $i$-th site. The functional form of $V$ is arbitrary, and the coefficient of hopping $t_i$ is position-dependent in general. The Hamiltonian of the head system

$$H_h = \sum_{i} t_i c_{i+1}^\dagger c_i + c.c. + V(n)$$

can be either integrable or chaotic. We remark that differently from the case with a single fermion the boundary condition is set as the periodic boundary condition.

In this system, a circle move of head particles represents the move of head particles that each particle moves to the position of the nearest rightmost particle in the present configuration. Take a case with $L = 5$ and $N = 2$ as an example (see Fig. 4). We label two fermions as A and B for convenience of explanation with keeping in mind that these two are in fact indistinguishable. Suppose that the fermion A is at the site 3, and the fermion B is at the site 5. The circle move of these head particles means the move of A as $3 \rightarrow 4 \rightarrow 5$ and B moves as $5 \rightarrow 1 \rightarrow 2 \rightarrow 3$. Then, a single circle move of head particles updates the state of the CA system by one step (See also Fig. 5, which depicts the case of $L = 9$ and $N = 3$). Remark that the rule of the classical CA emulated by this model is slightly different from the conventional one in that the update at the boundary refers states of $N$-step before and after. We call this classical CA as modified CA. We emphasize that this modified CA is still a classical CA, and to obtain the solution of this modified CA we need not to solve quantum fermion problems. Under this modified CA rule, $4^N$ possible states of the CA are decomposed into cycles, and we safely define the length of a cycle. Thus, by fixing a basing configuration of head particles and the initial state of the CA system on the $k$-th cycle, the state of the CA system at the $n$-th step ($0 \leq n \leq u_k - 1$) with the present configuration of the head system $\sigma$ is uniquely determined, which we denote by $|X_{k,\sigma}^n\rangle$.

Suppose that the state of the CA system belongs to the cycle $k$. Then, $u_k$-times circle moves of fermions in the head system convey the total system back to the original state. To reflect this fact, we depict as an example the state space in case of $L = 5$, $N = 2$, and $u_k = 3$ in Fig. 6. In this figure, we omit the details of the state of the CA system. The state space of only the head system (Fig. 6(a)) is extended by $u_k$ times, in which we can see the similarity to the case with a single fermion shown in Fig. 3.

To obtain the energy eigenstates of the total system $H$, we consider $H_h$, the Hamiltonian of only the head system with $2\pi s$ phase-twisted boundary condition. This boundary condition means that if a particle hops from the site $L$ to 1, then the phase $e^{2\pi si}$ is multiplied to the state. We denote by $|\Phi_j(s)\rangle$ the $j$-th energy eigenstate (1 $\leq j \leq a := \left(\frac{L}{2}\right)$) of $H_h$ with $2\pi s$ phase-twisted boundary condition. We also denote by $E_j(s)$ the corresponding eigenenergy. We expand $|\Phi_j(s)\rangle$ with spatial configurations as

$$|\Phi_j(s)\rangle = \sum_{\sigma} c_{\sigma}^j(s)|\sigma\rangle,$$
we cannot calculate $|\Phi_j(s)\rangle$ explicitly, while the formal solution of the total system is still given by Eq. (15), which is still helpful to discuss some properties of thermalization.

The trick of the eigenstates with the phase-twisted boundary condition have already been seen in the case with a single fermion in Sec. V. In this case, energy eigenstates and eigenenergies of the head system with no phase-twist is written as

$$|E_l\rangle = \frac{1}{\sqrt{L}} \sum_{i=1}^{L} e^{-\frac{2\pi il}{L}} |i\rangle$$

with $l = 0, 1, \ldots, L - 1$, which correspond to the case of $m = 0$, $u_k$, $2u_k$, $\cdots$, $(L - 1)u_k$ in Eqs. (7) and (8). Other solutions with other $m$s correspond to the solutions of the head system with phase-twist $2\pi i/u_k, 4\pi i/u_k, \ldots, 2(u_k - 1)\pi i/u_k$. The solutions with $m = 1$, $u_k + 1$, $2u_k + 1$, $\cdots$, $(L - 1)u_k + 1$ of Eq. (7), for example, correspond to energy eigenstates of the head system with $2\pi i/u_k$ phase-twisted boundary condition. The reason why phase-twist appears is as follows. A state of the head system goes back to the original state with a single circle move of fermions. In contrast, if the CA system is attached to the head system, the total state goes back to the original state with $u_k$ circle moves, and a single circle move not necessarily conveys the state to the original one. Hence, there is additional arbitrariness of the phase $2\pi i/u_k, 4\pi i/u_k, \cdots, 2(u_k - 1)\pi i/u_k$ per single circle move. This is the origin of the phase-twisted boundary condition.

**B. Analytic result of thermalization in this generalized model**

To construct a model of thermalization, we put assumptions on the modified classical CA as we do in Sec. V. Since the time evolution of the bulk of the modified CA is same as that of the conventional reversible CA, we assume that there exists a chaotic modified CA which satisfies the three conditions (thermalization, many cycles, no coherence) presented in Sec. V. In the following, we consider the emulation of this CA.

We now investigate some analytic properties of this quantum model. First, if the initial state of the CA system is not spatially-periodic in the modified sense (i.e., the state is spatially-periodic in the bulk and the boundary condition connecting $N$-step before keeps this periodicity), this system thermalizes. If the Hamiltonian of the head system $H_h$ is integrable, thermalization occurs only in the CA system as in the case of a single fermion. In contrast, if $H_h$ is chaotic, thermalization occurs not only in the CA system but in the total system.

Next, we consider the validity of the ETH. We first take a cycle of a classical conventional CA (not the modified CA) with the spatial period $r$. Then the length of this cycle must divide $(d^2r)!$ because the number of possible states with the spatial period $r$ is $d^2r$. Since the particle number diverges in the thermodynamic limit, we safely assume that $N$ is a multiple of $(d^2r)!$, which leads to $x_n^r = x_{n+N}^r$, $x_L^r = x_{L+N}^r$ for any $n$ in the classical conventional CA with the spatial period $r$. This directly implies the crucial fact that as for this cycle the conventional CA...
and the modified CA are completely the same. Hence the corresponding energy eigenstate of the quantum system has the spatial period \( r \), which is not a thermal energy eigenstate. We thus conclude that this quantum system does not satisfy the ETH.

We can also evaluate the effective dimension of some initial states. The dimension of the Hilbert space of the total system is \( D = D_{\text{head}} \cdot 2^{2L} \), where \( D_{\text{head}} \) is the dimension of the Hilbert space of the head system in the energy shell with the corresponding energy. We now calculate the effective dimension of the state \( |\sigma\rangle |X_k\rangle \), where \( |X_k\rangle \) is a state in the computational basis on the cycle \( k \). The functional form of the energy eigenstates \([15]\) suggests that the effective dimension of this state is bounded above by \( D_{\text{eff}} \leq D_{\text{head}} u_k \). Since \( u_k / 2^{2L} \) is exponentially small with respect to \( L \), we find that \( D_{\text{eff}} / D \) is exponentially small, and thus the thermalization of this model is not explained by the large effective dimension scenario.

### VII. DISCUSSION

We have introduced a quantum model that emulates a classical reversible CA. Differently from existing ideas of quantum CA \([49, 50]\) and quantum emulation of classical computation \([41]\), our model achieves emulation of stationary dynamics with a local and static Hamiltonian. With the help of the knowledge on the emulated classical CA, we can fully solve its energy eigenstates and eigenenergies, which gives a great advantage to our model. The level statistics of this model, for example, can be explicitly written down. In particular, emulation of a chaotic CA provides a solvable model of thermalization, which serves as a good stage to examine some existing scenarios of thermalization. Maybe surprisingly, although our model thermalizes, this thermalization cannot be explained by two leading scenarios, the ETH scenario and the large effective dimension scenario.

The violation of the ETH and thermalization coexist because we cannot sample non-thermal energy eigenstates in preparable initial states. Although completely spatially-periodic states do not thermalize, a single defect which destroys spatial periodicity is sufficient to induce thermalization and thermal noise inevitably causes defects. Essentially the same point has already been discussed in Refs. \([15, 16]\). This shows clear contrast to integrable systems where non-thermal energy eigenstates have negligibly small fraction, while physically plausible initial states can have exponentially heavy weight on these non-thermal energy eigenstates \([52]\).

### Acknowledgments

The author thanks Shinji Takesue for helpful advice on the reversible CA and Keisuke Fujii for fruitful discussion on quantum computation. The author also thanks Eiki Iyoda and Hiroyasu Tajima for useful comments. This work was supported by Grant-in-Aid for JSPS Fellows JP17J00393.

### Appendix A: Clarification of terminology

We here clarify some of terminology used in this paper. In case that a term does not have an undisputed definition and characterization, we put only some explanations on it.

**Integrable/non-integrable**: Although there is no undisputed definition of quantum (non-)integrability, in this paper we call a system non-integrable if the system has no local conserved quantity. If a system has some local conserved quantities, we call this system integrable. In this definition, an integrable system is not necessarily an exactly solvable system, which has sufficiently many local conserved quantities to determine each energy eigenstate. We note that a recent study \([53]\) succeeds in proving the non-integrability in a specific model, the XYZ chain with a magnetic field.

**Thermal state**: To give a precise definition of the thermal state in a macroscopic system, we first introduce a macroscopic observable (in a one-dimensional system). An observable \( A \) is called macroscopic observable if \( A \) is a sum of local observables \( A = \sum A_i \) (i.e., the support of \( A_i \) is contained by \( |i - r, i + r| \) with a fixed constant \( r \)). Then, a state \( |\Psi\rangle \) of a system \( X \) is thermal if any macroscopic observable \( A \) satisfies

\[
\lim_{L \to \infty} \langle \Psi | A | \Psi \rangle = \lim_{L \to \infty} \text{Tr}[A \rho^\text{mc}(X)],
\]

where \( \rho^\text{mc}(X) \) is a microcanonical ensemble of \( X \) with energy \( \langle \Psi | H | \Psi \rangle \). If a state \( |\Psi\rangle \) is thermal, then the partial trace to any subsystem with finite size \( X' \subset X \) turns to be the Gibbs state of this subsystem:

\[
\lim_{L \to \infty} \text{Tr}_{X \setminus X'} |\Psi\rangle \langle \Psi| = \lim_{L \to \infty} \text{Tr}_{X \setminus X'} |\rho^\text{mc}(X')\rangle.
\]

**Chaos**: We here elucidate a sharp difference between the case of few-body systems and many-body systems. In case of few-body systems, we can measure any observable of the system. The notion of few-body chaos is characterized on the basis of this fact. A classical few-body system is chaotic if for almost all initial states the long-time average of any Lebesgue measurable observable is equal to its ensemble average of microcanonical ensemble (i.e., ergodicity in the phase space). A quantum few-body system is chaotic if for all initial states the expectation value of any Lebesgue measurable observable after relaxation is equal to its ensemble average of microcanonical ensemble. In the quantum case, we keep \( \hbar \to 0 \) limit (semiclassical limit) in mind. We remark that (1) classical systems allow exceptional initial states with measure zero, (2) classical systems needs long-time average.
By contrast, in case of many-body systems, we can measure only macroscopic observables, not all observables. Therefore, the term thermal is defined with respect to macroscopic observables. In a similar manner, a classical many-body system is chaotic if for almost every initial state the long-time average of any macroscopic observable is equal to its ensemble average of microcanonical ensemble. A quantum many-body system is chaotic if for all initial states the expectation value of any macroscopic observable after relaxation is equal to its ensemble average of microcanonical ensemble. We emphasize that we do not require ergodicity in the phase space. In fact, no classical CA and no quantum many-body system show ergodicity in this sense. In many-body systems, the restriction of observable is crucial for characterization of thermalization and chaos.

We note that the Wigner-Dyson level statistics and quantum chaotic systems. For specialists, we remark that we use the definition of chaos, but frequently-appearing properties in thermalization and chaos.

We distinguish the diagonal ETH and the off-diagonal ETH. In this paper, we make correspondence between the function \( f(a, b, c) \) and an integer \( z \in \{0, 1, \cdots, 255\} \). The correspondence is given by

\[
z = \sum_{a,b,c} f(a, b, c) 2^{4a+2b+c}, \tag{B1}
\]

where \( a, b, \) and \( c \) take 0 or 1. For example, the rule 214 (= 128+64+16+8+4) describes the following transition rule:

| 111 | 110 | 101 | 100 | 011 | 010 | 001 | 000 |
|-----|-----|-----|-----|-----|-----|-----|-----|
| 1   | 1   | 0   | 1   | 1   | 1   | 0   | 0   |

Appendix C: Precise statement of the conditions on a chaotic CA

We here present the precise statement of the three conditions on a chaotic CA explained in Sec. [V]

(i) We fix a finite \( l \), and consider \( 2(l+1) \) sites in \( C_{i,i+l} \). Let \( s_{i,i+l}^n \) be a state of \( C_{i,i+l} \) at the \( n \)-th step. We require that for any cycle \( k \) with no spatial periodicity and for any states of \( C_{i,i+l} \) denoted by \( y \in (S_d)^{2(l+1)} \), the following relation

\[
\lim_{L \to \infty} \sum_{n=1}^{u_k} \frac{\chi(s_{i,i+l}^n = y)}{u_k} = \frac{1}{d^{2(l+1)}} \tag{C1}
\]

does not satisfy, where \( \chi(\cdot) \) takes one if the statement in the clause is true and takes zero otherwise.

(ii) We require that the maximum length of a cycle is exponentially small compared to the number of possible states:

\[
-\lim_{L \to \infty} \frac{1}{L \ln \frac{\max_k u_k}{d^L}} \neq 0. \tag{C2}
\]

(iii) We fix a finite \( l \), and consider states of \( 2(L-l+1) \) sites in \( C_{i,i+l-l} \) which we denote by \( s_{i,i+l-l}^n \). For any cycle \( k \), we construct a subset of \( \{1, 2, \cdots, u_k\} \) as

\[
D_k = \{ n \mid \exists n' \neq n \text{ s.t. } s_{i,i+l-l}^n = s_{i,i+l-l}^{n'} \}. \tag{C3}
\]

We require that the size of \( D_k \) is negligibly small:

\[
\lim_{L \to \infty} \max_k \frac{|D_k|}{u_k} = 0. \tag{C4}
\]

Appendix D: Large effective dimension scenario

We here give a precise statement on the fact that the large effective dimension ensures the existence of thermalization, which is discussed in Sec. [V] and Sec. [VI]. We first fix the precision \( \delta > 0 \). Let \( P^\delta_{eq} \) be a projection operator onto the nonequilibrium subspace where there is a macroscopic observable whose density is different from the corresponding microcanonical average by more than \( \delta \). Ordinal thermodynamic system satisfies

\[
\text{Tr}[P^\delta_{eq} P^{mc}] \leq e^{-\gamma(\delta)L} \tag{D1}
\]

for any large \( L \), which exhibits the large deviation property of the microcanonical ensemble. Here, \( \gamma(\delta) \) is independent of \( L \), and it converges to zero as \( \delta \to 0 \). A state \( \langle \Psi \rangle \) thermalizes with precision \( \delta \) if \( \langle \Psi | P^\delta_{eq} | \Psi \rangle \) converges to zero in the thermodynamic limit.

It is shown that thermalization with precision \( \delta \) indeed occurs if the effective dimension of the initial state satisfies

\[
D_{eff} \geq e^{-\gamma(\delta)L} \delta \tag{D2}
\]
with $\gamma(\delta)$ given in Eq. [D1]. Since we should adopt the case of the perfect precision limit $\delta \to 0$ as an ideal limit, the above result can be interpreted as that thermalization is confirmed if $D_{\text{eff}}/D$ decays slower than any exponential function of $L$ in the thermodynamic limit.

[1] T. Kinoshita, T. Wenger, and D. S. Weiss, A quantum Newton’s cradle. Nature 440, 900 (2006).
[2] M. Cramer, A. Flesch, I. P. McCulloch, U. Schollwöck, and J. Eisert, Exploring Local Quantum Many-Body Relaxation by Atoms in Optical Superlattices. Phys. Rev. Lett. 101, 063001 (2008).
[3] M. Gring, M. Kuhnert, T. Langen, T. Kitagawa, B. Rauer, M. Schreitl, I. Mazets, D. Adu Smith, E. Demler, and J. Schmiedmayer, Relaxation and Prethermalization in an Isolated Quantum System, Science 337, 1318 (2012).
[4] M. Rigol, V. Dunjko, M. Olshanii, Thermalization and its mechanism for generic isolated quantum systems. Nature 452, 854 (2008).
[5] T. Langen, S. Erne, R. Geiger, B. Rauer, T. Schweigler, M. Kuhnert, W. Rohringer, I. E. Mazets, T. Gasenzer, and J. Schmiedmayer, Experimental observation of a generalized Gibbs ensemble. Science 348, 207 (2015).
[6] P. Essler and M. Fagotti, Quench dynamics and relaxation in isolated integrable quantum spin chains. J. Stat. Mech. 064002 (2016).
[7] R. Steinigeweg, J. Herbrych, and P. Prelovšek, Eigenstate thermalization within isolated spin-chain systems. Phys. Rev. E 87, 012118 (2013).
[8] H. Kim, T. N. Ikeda, and D. A. Huse, Testing whether all eigenstates obey the eigenstate thermalization hypothesis. Phys. Rev. E 90, 052105 (2014).
[9] W. Beugeling, R. Moessner, and M. Haque, Finite-size scaling of eigenstate thermalization. Phys. Rev. E 89, 042112 (2014).
[10] L. F. Santos, A. Polkovnikov, and M. Rigol, Entropy of Isolated Quantum Systems after a Quench. Phys. Rev. Lett. 107, 040601 (2011).
[11] M. Rigol, Fundamental Asymmetry in Quenches Between Integrable and Nonintegrable Systems. Phys. Rev. Lett. 116, 100601 (2016).
[12] M. C. Bañuls, J. I. Cirac, and M. B. Hastings, Strong and Weak Thermalization of Infinite Nonintegrable Quantum Systems, Phys. Rev. Lett. 106, 050405 (2011).
[13] H. Kim, M. C. Bañuls, J. I. Cirac, M. B. Hastings, and D. A. Huse, Slowest local operators in quantum spin chains, Phys. Rev. E 92, 012128 (2015).
[14] J. von Neumann, Beweis des Ergodensatzes und des H-Theorems in der neuen Mechanik. Z. Phys. 57, 30 (1929) [English version, Proof of the ergodic theorem and the H-theorem in quantum mechanics, Eur. Phys. J. H 35, 201 (2010)] .
[15] H. Tasaki, From Quantum Dynamics to the Canonical Distribution: General Picture and a Rigorous Example. Phys. Rev. Lett. 80, 1373 (1998).
[16] P. Reimann, Foundation of Statistical Mechanics under Experimentally Realistic Conditions. Phys. Rev. Lett. 101, 190403 (2008).
[17] N. Linden, S. Popescu, A. J. Short, and A. Winter, Quantum mechanical evolution towards thermal equilibrium. Phys. Rev. E 79, 061103 (2009).
[18] C. Gogolin, M. P. Müller, and J. Eisert, Absence of Thermalization in Nonintegrable Systems. Phys. Rev. Lett. 106, 040401 (2011).
[19] A. J. Short and T. C. Farrelly, Quantum equilibration in finite time. New J. Phys. 14, 013063 (2012).
[20] G. De Palma, A. Serafini, V. Giovannetti, and M. Cramer, Necessity of Eigenstate Thermalization, Phys. Rev. Lett. 115, 220401 (2015).
[21] C. Gogolin and J. Eisert, Equilibration, thermalisation, and the emergence of statistical mechanics in closed quantum systems. Rep. Prog. Phys. 79, 056001 (2016).
[22] T. Farrelly, F.G.S.L. Brandao, M. Cramer, Thermalization and Return to Equilibrium on Finite Quantum Lattice Systems. Phys. Rev. Lett. 118, 140601 (2017).
[23] L. P. Garca-Pintos, N. Linden, A. S.L. Malabarba, A. J. Short, and A. Winter, Equilibration Time Scales of Physically Relevant Observables. Phys. Rev. X 7, 031027 (2017).
[24] I. Affleck, T. Kennedy, E. H. Lieb, and H. Tasaki, Rigorous results on valence-bond ground states in antiferromagnets, Phys. Rev. Lett. 59, 799 (1987).
[25] P. Gacs. Reliable Cellular Automata with Self-Organization. J. Stat. Phys. 103, 45 (2001).
[26] T. S. Cubitt, D. Perez-Garcia, and M. M. Wolf, Undecidability of the spectral gap. Nature 528, 207 (2015).
[27] R. Movassagh and P. W. Shor. Supercritical entanglement in local systems: Counterexample to the area law for quantum matter. Proc. Nat. Acad. Sci. 113, 13278 (2016).
[28] F. Haake, Quantum Signatures of Chaos, Springer (2010).
[29] M. V. Berry, Semiclassical Theory of Spectral Rigidity. Proc. R. Soc. London, Ser. A 400, 229 (1985).
[30] M. Sieber and K. Richter, Correlations between periodic orbits and their role in spectral statistics. Physica Scripta, T90, 128 (2001).
[31] S. Müller, S. Heusler, P. Braun, F. Haake, and A. Altland, Semiclassical Foundation of Universality in Quantum Chaos. Phys. Rev. Lett. 93, 014103 (2004).
[32] T. Kottos and U. Smilansky, Periodic Orbit Theory and Spectral Statistics for Quantum Graphs. Ann. Phys. 274, 16 (1999).
[33] G. Berkolaiko, H. Schanz, and R. S. Whitney, Leading Off-Diagonal Correction to the Form Factor of Large Graphs. Phys. Rev. Lett. 88, 104101 (2002).
[34] M. C. Gutzwiller, Periodic Orbits and Classical Quantization Conditions. J. Math. Phys. 12, 343 (1971).
[35] J. H. Hannay and A. M. Ozorio De Almeida, Periodic orbits and a correlation function for the semiclassical density of states. J. Phys. A 17, 3429 (1984).
[36] H. Tasaki, Typicality of Thermal Equilibrium and Thermalization in Isolated Macroscopic Quantum Systems. J. Stat. Phys. 163, 937 (2016).
[37] S. Wolfram, A New Kind of Science. Wolfram media inc (2002).
[38] S. Takesue, Ergodic properties and thermodynamic behav-
ior of elementary reversible cellular automata. I. Basic properties. J. Stat. Phys. 56, 371 (1989).

Let $r$ be a divisor of $L$. Suppose that for any $i, j$ satisfying $i \equiv j \mod r$, the relation $x_i^n = x_j^n$ holds for $n = 1, 2$. Then the above relation holds for any $n$.

We here put two remarks. First, although the state space is separated in a particular way, the conventional GGE does not appear to describe the CA system after relaxation. This is because the separation is not characterized by a local conserved charge. Second, owing to the head system there exists some trivial local conserved quantities. Thus, relaxation occurs in each sector characterized by these local conserved quantities. However, fortunately, all sectors give the same expectation values of observables in the CA system, which enables us to say that these conserved quantities are harmless and the relaxation in each sector is also thermalization.

J. M. Deutsch, Quantum statistical mechanics in a closed system. Phys. Rev. A 43, 2046 (1991).

M. Srednicki, Chaos and quantum thermalization. Phys. Rev. E 50, 888 (1994).

M. Horoi, V. Zelevinsky, and B. A. Brown, Chaos vs Thermalization in the Nuclear Shell Model. Phys. Rev. Lett. 74, 5194 (1995).

N. Shiraishi and T. Mori, Systematic Construction of Countereamples to Eigenstate Thermalization Hypothesis. Phys. Rev. Lett. 119, 030601 (2017).

T. Mori and N. Shiraishi, Thermalization without eigenstate thermalization hypothesis after a quantum quench. Phys. Rev. E 96, 022153 (2017).

S. Goldstein, T. Hara, and H. Tasaki, The approach to equilibrium in a macroscopic quantum system for a typical nonequilibrium subspace, arXiv:1402.3380 (2014)

We remark that diverging $D_{\text{eff}}$ only implies relaxation to some stationary state, and even exponentially large $D_{\text{eff}} = O(e^L)$ but $D_{\text{eff}}/D = O(e^{-L})$ is seen in non-thermalizing systems including integrable systems [11]. In other words, to guarantee thermalization solely by the largeness of effective dimension, $D_{\text{eff}}/D = \text{poly}(1/L)$ is necessary.

C. S. Lent, P. D. Tougaw, W. Porod, and G. H. Bernstein, Quantum cellular automata. Nanotechnology 4, 49 (1993).

B. Schumacher, R.F. Werner, Reversible quantum cellular automata. arXiv:quant-ph/0405174 (2004).

R. Feynman, Quantum mechanical computers. Optics News 11, 11 (1985).

G. Biroli, C. Kollath, and A. M. Läuchli, Effect of Rare Fluctuations on the Thermalization of Isolated Quantum Systems. Phys. Rev. Lett. 105, 250401 (2010).

N. Shiraishi, Proof of the absence of local conserved quantities in the XYZ chain with a magnetic field. arXiv:1803.02637 (2018).

N. Shiraishi and T. Mori, Shiraishi and Mori Reply. arXiv:1712.01999 (2017).