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Steady State of Closed Integrable Systems
（閉じた可積分系の定常状態）

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Abstract

In the present thesis, we consider the long-time steady state of closed many-body quantum systems with integrability. Integrable systems have many conserved quantities. One of our aims is to clarify the role of those conserved quantities in relaxation.

This thesis consists of two parts. In the first part, we consider the steady state of static integrable systems. We formulate a generalization of the eigenstate thermalization hypothesis (ETH), which is a sufficient condition for equilibration to the Gibbs state under unitary evolution. We analytically prove the validity of the generalized ETH for translationally invariant noninteracting integrable systems. This leads to the validity of the generalized Gibbs ensemble (GGE), which was proposed to describe the steady state of integrable systems. We expect the generalized ETH to be the general mechanism of relaxation of integrable systems to a steady state described by the GGE.

In the second part, we consider the steady state of closed systems whose Hamiltonian changes periodically in time, namely time-periodic systems. Time-periodic systems can be analyzed by the Floquet theory, in which an effective Hamiltonian for the unitary evolution over one period plays the central role. We consider time-periodic systems whose effective Hamiltonian is integrable. We numerically study in detail the heating behavior of integrable time-periodic systems. We find that heating to high temperatures can occur in integrable time-periodic systems, which is a nontrivial result in the context of preceding discussions. We find a scaling behavior as to the heating in the low-frequency regime. We also study the steady state from the viewpoint of a generalized Gibbs ensemble for time-periodic systems. We also discuss the origin of heating in the present systems.

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List of Publications

This thesis is based on the following papers:

1. Takashi Ishii, Tomotaka Kuwahara, Takashi Mori, and Naomichi Hatano. Heating in integrable time-periodic systems. *Phys. Rev. Lett.*, 120:220602, May 2018.

2. Takashi Ishii and Takashi Mori. Strong eigenstate thermalization within a generalized shell in noninteracting integrable systems. *arXiv preprint arXiv:1810.00625*, 2018.

Contents

Chapter 1

Introduction

1.1 Thermalization

Thermalization [1–3] is one of the fundamental principles of thermodynamics. Its statement can be made in twofolds: first, a macroscopic isolated system without external operations imposed relaxes to a steady state whose macroscopic properties do not change thereafter. This is called equilibration or relaxation. Second, thermalization implies that the steady state can be described by only a small number of quantities, e.g., the energy, the density, the magnetization, and so on.

The surprisingly wide universality of thermodynamics has been confirmed by numerous experiments, which were conducted from the very early years for gases [4]. One may also perceive that thermalization is observed in many occasions in everyday life too. However, the explanation of thermalization from microscopic mechanics has not been achieved yet. When we consider this issue, we notice that this phenomenon is quite nontrivial from a microscopic point of view. Let us here introduce two points frequently pointed out in explaining in what sense it is nontrivial. Firstly, equilibration is already a nontrivial phenomenon, because while it is an irreversible phenomenon, the microscopic mechanics is reversible, whether in the classical or quantum case. It is well known that Boltzmann could not completely resolve this issue. The second point is on the validity of the simple description of the thermal equilibrium state by a small number of quantities. Macroscopic systems have an enormous number of degrees of freedom, e.g., a spin system with N pieces of two-components spins has a state space of the dimensionality 2^N. It is nontrivial how all properties of the thermal equilibrium state can be described by only a small number of quantities, despite the large dimensionality of the state space.

In statistical mechanics, it is presupposed that the thermal state is given by statistical ensembles characterized by only a few extensive variables, for example, the microcanonical ensemble, the canonical ensemble, and the grandcanonical ensemble, which are all equivalent in the thermodynamic limit. Given the established success of statistical mechanics, the issue of explaining thermalization by microscopic mechanics can be recasted as the question of validating the equilibration to the above statistical ensembles. However, the clarification of the generality and the microscopic mechanism of the validity of such statistical ensembles as a successful description of the thermal equilibrium state is still a problem which remains to be solved.

The study on the validation of the microcanonical ensemble in an isolated system has a long history. In the case of classical mechanics, the microcanonical ensemble is defined as the uniformly mixed state within a constant-energy surface. As for its validation, the ergodicity [5], as well as chaos [6] as a related subject, were considered. The ergodicity is stated as a property of the time evolution of a system: a state travels around all the region of the constant-energy surface with uniform probability in the long time-scale. If this property was satisfied, the long-time average of physical quantities equals that of the microcanonical ensemble. The ergodicity is mathematically proved for a few specific systems, such as the Sinai billiards [7] and the Bunimovich stadium [8]. Chaos is roughly speaking a characteristic complicated behavior of dynamics seen in a wide class of classical systems. Although there is no definite definition of chaos [2], usually the high sensitivity of the time evolution in the phase space to the initial state is considered as the main characteristic of systems regarded as chaotic. This sensitivity can be quantified by the Lyapnov exponent. Among other peculiar characteristics is the nonlinearity of the system.

However, as for ergodicity, it has been argued that since the time it takes for a large system to evolve in a sufficiently wide region of the phase space is extremely long, the ergodicity is not an adequate explanation of thermalization, which is observed in experimental timescales [9, 10]. In fact, the former timescale is estimated to be much longer than the age of the universe in systems with particle numbers of order 10^{23} [9, 10].

Also, of course it is now established that the microscopic mechanics of nature is quantum mechanics. However, the way of constructing possible quantum counterparts of ergodicity and chaos is not straightforward [2], although the terms “quantum ergodicity” and “quantum chaos” are frequently used. An apparent incompatibility of chaos with quantum mechanics was clear from its early days [2]; there is no nonlinearity in the Schrödinger equation.

Meanwhile, the explanation of thermalization in terms of quantum mechanics has also been considered from its early days. Schrödinger already considered this issue [11]. Von Neumann carried out a pioneering work on this issue [12]. For a while since then, study on the foundation of thermalization seems to have been of relatively low interest. However, it has gained great attention again in recent years. (Indeed, von Neumann’s work also gained renewed attention recently.) This is mainly due to the circumstances explained in the following.

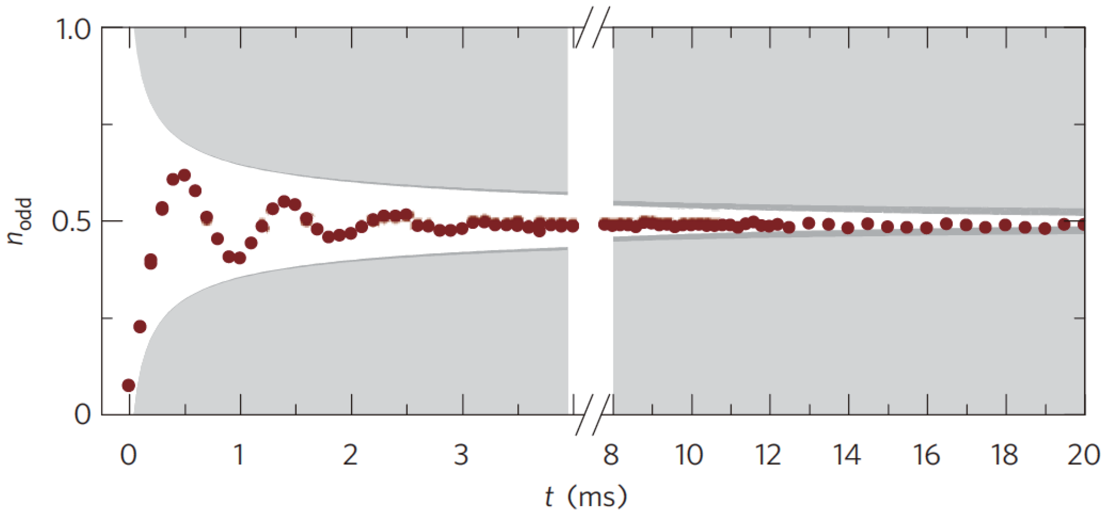


Figure 1.1: Experimental observation of thermalization by Trozky and coworkers [13]. At initial time, every even site of a one-dimensional optical lattice is occupied by one ^{87}Rb atom. The time evolution thereafter is governed by a nonintegrable Bose-Hubbard Hamiltonian. The number density at odd sites n_{odd} is shown to thermalize after enough time. Adapted from Fig. 1 of Ref. [13]. Copyright (2012) Springer Nature.

In recent years, owing to the remarkable progress in experimental techniques, the direct capturing of the unitary dynamics of isolated many-body systems has become available [13–16]. Systems that can be accounted to be isolated within the experimental timescale can be realized by using ultracold atoms and optical lattices now. It has been confirmed that thermalization indeed takes place in unitary evolution. Trotzky and coworkers [13] observed thermalization in a system of ultracold ^{87}Rb atoms in a one-dimensional optical lattice. They prepared the initial state as such that every even site is occupied by one ^{87}Rb atom, and quenched the system to a nonintegrable Bose-Hubbard Hamiltonian. They observed the time evolution of the number density at odd sites and showed that it thermalizes (see Fig. 1.1). Numerical simulation of isolated many-body systems with relatively large sizes has also become possible recently thanks to the improvement of numerical powers [17–19]. Studies of the relaxation and the steady state of isolated systems are actively done in recent years owing to these circumstances.

Recently, a concept called the typicality [9, 10, 20–27] is actively discussed, mainly in the quantum regime, as a presumably adequate way of understanding thermalization. The typicality is a statement on the states in the state space where the dynamics takes place. Roughly, it states that almost all microscopic states within the state space cannot be distinguished macroscopically from each other, and moreover, from the thermal state. According to this concept, thermalization of a state initially out of equilibrium can be explained as a process in which a macroscopically atypical initial microstate evolves in time and gradually enters the region of the state space where the microstates are macroscopically typical. This explanation is successful in avoiding the aforementioned criticism on the discussion of ergodicity.

A rough explanation of some specific formulations of the typicality, rigorously proved in [10, 21, 26, 27] is as follows. In quantum mechanics, the microcanonical ensemble is defined as a mixed state with equal weight put on all eigenstates within an energy shell. For several systems, it was proved that almost all microstates given as a superposition of the eigenstates in the energy shell are macroscopically indistinguishable from the microcanonical ensemble. The crucial point is to restrict observables under consideration to "physical" ones. Frequently used definitions of "physical" observables are few-body observables or spatially local observables, e.g., few-body or spatially local correlations and reduced density matrices for a finite region of the system. This allows one to regard two microscopically different states as being indistinguishable.

However, although the concept of typicality greatly helps in understanding thermalization as well as the recently proposed eigenstate thermalization hypothesis (ETH), which we will explain below, the connection between the atypical or typical states and the states which appear in the initial preparation or time evolution in realistic dynamics has not been resolved. A paradigm of dynamics that has been studied extensively and considered as one of such realistic dynamics is the quench. Quench is a dynamics where the initial state is usually the ground state $|\psi_0\rangle$ or a low-temperature Gibbs state of an ordinary Hamiltonian H_0, and at a time $t = 0$, the Hamiltonian is switched to another Hamiltonian H, which governs the following dynamics. It may seem adequate to assume that in the case of quench for a ground state $|\psi_0\rangle$, states at late times are given by typical states in the energy shell around $E = \langle\psi_0|H|\psi_0\rangle$. Likewise we may be able to assume that the states at late times after a realistic dynamics are given by typical states in a relevant state space. However, this is only an intuitive discussion; typicality does not suffice to prove thermalization rigorously.

Recently, a hypothesis called the eigenstate thermalization hypothesis (ETH) has been proposed [18, 28, 29]. Roughly speaking, it states that all individual eigenstates have the thermal property. We note that ETH can be considered in a way as a manifestation of a quantum analogue of chaos [2]. The ETH is a sufficient condition for thermalization as will be explained in detail in Chap. 3. The ETH constitutes a central topic in Part I of this thesis, together with the integrability, which we explain in Sec. 1.3.

1.2 Equilibration in closed time-periodic systems

While the validation of thermalization in static systems is a question which still remains to be solved as explained in the previous section, it is also an intriguing problem to explore the long-time behavior of systems whose Hamiltonian changes in time. Systems with time-periodic modulation is perhaps the simplest case of such systems.

The study on the properties of time-periodic systems has a long history too [30]. In time-periodic systems, interesting phenomena, such as dynamical phase transition [31–35], may take place even in the classical one-body regime [36, 37]. Vigorous exploring of the quantum many-body regime started recently [1, 30, 38–40].

While we consider the steady state of closed systems reached after unitary time evolution due to a static Hamiltonian in Part I of this thesis, we consider in Part II the steady state of closed but time-periodic systems in the quantum many-body regime. The dynamics of the system is given by the time-dependent Schrödinger equation. The properties of the long-time steady state of such systems are generally nontrivial because they are beyond the framework of usual equilibrium statistical mechanics.

A notable property of time-periodic systems is that the usual energy conservation does not hold, and thus a rise in energy, in other words the heating, may occur [41–43]. This can be understood that the system absorbs energy from the external driving. Heating can be understood as the relaxation towards the maximum entropy state in the whole Hilbert space [37, 44–47], and therefore it is also an issue of thermalization.

As we will see in sec. 6.2, time-periodic systems can be analyzed by the Floquet theory [30]; time-periodic systems can be mapped to the problem of a static system whose effective Hamiltonian is defined from the unitary operator over one driving period. However, we should keep in mind that such an effective Hamiltonian might differ greatly from Hamiltonians of usual thermodynamic systems; for example, the locality and the few-body properties of the interaction may be violated. On the other hand, this leads to the possibility of paving ways to interesting phenomena that cannot be achieved at least easily by usual static Hamiltonians [45, 46, 48–53] . Since time periodic systems are also relatively easy to be realized in experiments, it is studied actively in recent years both theoretically [31–35, 54–75] and experimentally [76–80] for the purpose of utilizing possible nontrivial phenomena. For example, the realization of a topological insulator by inducing a simple time-periodic external field on a topologically trivial matter was proposed [49, 59–64, 68, 71, 72, 75–78, 81]. This is called the Floquet topological insulator and its study is now beginning to flourish as a distinct field of research. To name other few, the control of phase transition from the superfluid to a Mott-insulator was predicted [82] and later observed in an experiment [83]; the detection of Higgs mode in superconductors was achieved [79]. However, the heating may break interesting physical phases, so that it is a serious problem that one wants to avoid. Therefore, the clarification of the general condition and extent of heating is desired also in the field of applications.

1.3 Integrability

It is known that integrability plays a crucial role in equilibration; this will be explained in the next subsection. Besides the role in equilibration, integrable systems possess a particular importance in theoretical studies because rigorous analysis to a substantial extent is usually possible in integrable systems. Integrable systems frequently appear in theories, e.g., as approximated models of realistic systems.

Let us here explain the definition of integrability [84]. In classical mechanics, there is a clear definition of integrability: a system with N degrees of freedom is said to be integrable when there are N independent constants of motion. However, there is no generally established definition of integrability in quantum systems. A tentative definition can be proposed: a system is said to be integrable when there are N independent operators that commute with the Hamiltonian H. However this definition has a serious problem as follows. Consider the spectral decomposition of an arbitrary Hamiltonian as $H = \sum_{i=1}^{D} \lambda_i |\psi_i\rangle\langle\psi_i|$, where D is the dimensionality of the Hilbert space while λ_i and $|\psi_i\rangle$ are the eigenvalues and eigenvectors, respectively. Each of the projections $|\psi_i\rangle\langle\psi_i|$ is an operator that commutes with H, and there are D of them. Thus, an arbitrary Hamiltonian satisfies the above tentative definition, unless one somehow specifies the class of commuting operators to be considered. Nevertheless, there seems to be a vague consensus as to which system is integrable and which is not, and the above sort of tentative definition is common in the literature.

In the present thesis, specific analysis is made for systems which are written in the quadratic form of fermions. Such systems form a class of integrable systems, and is said to be noninteracting in the sense that they can be mapped to free fermions. The extension of our analysis to interacting integrable systems (which are solved by the Bethe ansatz [85]) is left as future works. Let us note beforehand that while noninteracting integrable systems are simple compared to interacting ones, they are not necessarily less important as a subject to be studied. We expect that our results have opened ways to understanding also the case of general integrable systems, and may also (especially for the result of Part I) provide insights for the case of nonintegrable systems; more specific comments on this point will be made in the Conclusions.

1.3.1 Equilibration in the presence of integrability

Static systems

Thanks to the great advances in experimental techniques on optical lattices and cold atoms already mentioned in Sec. 1.1, it is now possible to experimentally realize systems described by integrable models, and its dynamical properties as well as the properties of the steady state have been observed [86]. The study of the relaxation and the steady state of integrable systems constitutes a large field in the recently active theoretical and experimental researches on isolated systems.

It is known that in integrable systems the steady state generally does not coincide with the usual Gibbs state [87–90]. This can be understood as a consequence of the presence of the conserved quantities, because they restrict the dynamics in the Hilbert space. It was recently proposed [87] that the steady states of integrable systems are given instead by a statistical ensemble called the generalized Gibbs ensemble (GGE). The GGE can be considered as a generalization of the usual Gibbs ensemble, and is constructed with many conserved quantities of the system. We give detailed explanation of the GGE in Chapter 4.

Time-periodic systems

Time-periodic systems can be classified into nonintegrable or integrable systems too depending on the integrability of its effective Hamiltonian. In the case of integrable time-periodic systems, the conserved quantities of the effective Hamiltonian restrict the dynamics. As for integrable time-periodic systems, understanding of the steady state, in particular the extent of heating, has been limited (See Sec. 7.2.) compared to nonintegrable time-periodic systems (See Sec. 6.3.). Its general understanding is an important problem because integrable time-periodic models are adopted in analyses of time-periodic systems, and are also expected to be realizable experimentally by means of current techniques of time-periodic modulation of optical lattices and ultracold atoms [80].

As we will see in Sec. 7.3, it has been proposed [53] that the steady state of integrable time-periodic systems is given by a form of GGE, namely the Floquet GGE. However, we note that we should be cautious not to apply discussions on static systems carelessly to time-periodic systems, because the effective Hamiltonian of time-periodic systems generally does not satisfy properties which usual static Hamiltonian has, such as the locality of interactions, as mentioned in Sec. 1.2. The validity of the description of the steady state of integrable time-periodic systems in terms of the GGE is unclear compared to the case of static integrable systems.

1.4 The organization of this thesis

The organization of this thesis is as follows.

In Part I, we first review prior understanding on equilibration and thermalization, and then on the steady state of integrable systems. In the sections thereafter we construct a microscopic mechanism for the description of steady states of integrable systems in terms of the GGE and analytically prove its validity for noninteracting integrable systems. The precise organization of Part I is as follows. In Chapter 2 we review a recently presented theoretical explanation of equilibration under unitary evolution. In Chapter 3 we review the eigenstate thermalization hypothesis (ETH), which was proposed as a mechanism of the steady state reached after a long time being described by the Gibbs ensemble. In particular, we stress that while a variant of the ETH, namely the *weak ETH*, has been proposed, only the ETH guarantees thermalization, whereas the weak ETH does not. In Chapter 4 we review the generalized Gibbs ensemble (GGE), which was proposed and also proved under certain limited conditions as the description of the steady state of integrable systems. In Chapter 5 we formulate and prove a mechanism of the relaxation to GGE in translationally invariant noninteracting integrable systems.

The organization of Part II is as follows. We give a review of time-periodic systems in Chapter 6. We give further explanation in the case of integrable time-periodic systems in Chapter 7. In Chapter 8 we consider a specific integrable time-periodic system and numerically study its heating behavior in detail. We clarify that heating to the high temperature may take place in integrable time periodic systems too. We also reveal for our models that in the limit of the system size and driving period tending to infinity, the energy of the steady state coincides with that of the infinite-temperature state. We also discuss the condition under which heating to the high temperature takes place in the present integrable models.

In Chapter 9 we make a summary and present future perspectives.

Part I

Description of the steady state and its mechanism in static integrable systems

Chapter 2

Relaxation of static systems under unitary evolution

We here review a theoretical explanation [91] of the equilibration of isolated many-body quantum systems under unitary evolution of a static Hamiltonian, following [92]. We set $\hbar = 1$ throughout this thesis. Denoting $|\alpha\rangle$ for $\alpha = 1, \ldots, D$ as the eigenstate of the Hamiltonian $\hat{H}$, where D is the dimensionality of the Hilbert space, the expectation value of the observable $\hat{o}$ for the state at time t, denoted as

$$|\psi(t)\rangle = \sum_\alpha C_\alpha e^{-iE_\alpha t}|\alpha\rangle, \tag{2.1}$$

is given by

$$\langle\psi(t)|\hat{o}|\psi(t)\rangle = \sum_{\alpha,\alpha'} C^*_{\alpha'} C_\alpha e^{-i(E_\alpha - E_{\alpha'})t}\langle\alpha'|\hat{o}|\alpha\rangle, \tag{2.2}$$

where E_α denotes the energy eigenvalue of $|\alpha\rangle$ and the initial state is $|\psi_0\rangle = \sum_\alpha C_\alpha|\alpha\rangle$. We hereafter assume that there is no energy degeneracy for simplicity. In the case where energy degeneracy exists, we can always choose an energy eigenbasis depending on the initial state, in which only one eigenstate for each distinct energy has nonzero overlap with the initial state; the eigenstate $|E\rangle$ for energy E is given by $|E\rangle = \sum_{\alpha \text{ s. t. } E_\alpha = E} C_\alpha|\alpha\rangle / \sqrt{\sum_{\alpha' \text{ s. t. } E_{\alpha'} = E} |C_{\alpha'}|^2}$. Then, the initial state can be written as $|\psi_0\rangle = \sum_\alpha v_E|E\rangle$, where $v_E \equiv \langle E|\psi_0\rangle$, and parallel arguments apply in the following. We note that we do not require this assumption in our analysis in Chap. 5.

The long-time average of $\langle\hat{o}\rangle \equiv \langle\psi(t)|\hat{o}|\psi(t)\rangle$ is given by

$$\begin{aligned}
\overline{\langle\hat{o}\rangle} &= \sum_{\alpha,\alpha'} C^*_{\alpha'} C_\alpha \langle\alpha'|\hat{o}|\alpha\rangle \overline{e^{-i(E_\alpha - E_{\alpha'})t}} && (2.3)\\
&= \sum_\alpha |C_\alpha|^2 \langle\alpha|\hat{o}|\alpha\rangle && (2.4)\\
&= \mathrm{Tr}[\rho_{DE}\hat{o}], && (2.5)
\end{aligned}$$

where the overline denotes the long-time average $\overline{f(t)} = \lim_{T\to\infty} \frac{1}{T}\int_0^T f(t)dt$, and $\rho_{DE} \equiv \sum_\alpha |C_\alpha|^2|\alpha\rangle\langle\alpha|$ is called the diagonal ensemble. In the following we prove under an assumption that the fluctuation of $\langle\hat{o}\rangle$ vanishes in the limit $D\to\infty$.

The assumption is the nondegeneracy in energy gaps:

$$E_k - E_l = E_m - E_n \Rightarrow \begin{cases} (E_k = E_l \text{ and } E_m = E_n) \\ \text{or} \\ (E_k = E_m \text{ and } E_l = E_n). \end{cases} \tag{2.6}$$

Under this assumption, we shall prove

$$\overline{(\langle\hat{o}\rangle - \overline{\langle\hat{o}\rangle})^2} \leq \frac{||\hat{o}||^2}{D_{\text{eff}}}, \tag{2.7}$$

where $||\cdot||$ is the operator norm and

$$D_{\text{eff}} \equiv \frac{1}{\sum_\alpha |c_\alpha|^4}. \tag{2.8}$$

The value D_{eff} is called the effective dimension. Note that $1 \leq D_{\text{eff}}$ and that $D_{\text{eff}} = d$ when the initial state has equal weight over d different energies. We can expect that $D_{\text{eff}} = e^{O(V)}$ [93]. Denoting $o_{\beta\alpha} \equiv \langle\beta|\hat{o}|\alpha\rangle$, we can rewrite Eq. (2.2) as

$$\langle\psi(t)|\hat{o}|\psi(t)\rangle = \sum_{\alpha\beta} C_\beta^* C_\alpha e^{-i(E_\alpha - E_\beta)t} o_{\beta\alpha}. \tag{2.9}$$

The difference of $\langle\hat{o}\rangle$ and $\overline{\langle\hat{o}\rangle}$ is

$$\langle\hat{o}\rangle - \overline{\langle\hat{o}\rangle} = \sum_{\substack{\alpha\beta \\ \alpha\neq\beta}} C_\beta^* C_\alpha e^{-i(E_\alpha - E_\beta)t} o_{\beta\alpha}. \tag{2.10}$$

We can calculate the fluctuation as

$$\overline{(\langle\hat{o}\rangle - \overline{\langle\hat{o}\rangle})^2} = \overline{|\langle\hat{o}\rangle - \overline{\langle\hat{o}\rangle}|^2} \tag{2.11}$$

$$= \overline{\sum_{\substack{\alpha\beta \\ \alpha\neq\beta}} \sum_{\substack{\gamma\delta \\ \gamma\neq\delta}} C_\beta^* C_\alpha C_\delta C_\gamma^* e^{-i(E_\alpha - E_\beta - (E_\gamma - E_\delta))t} o_{\beta\alpha} o_{\delta\gamma}^*} \tag{2.12}$$

$$= \sum_{\substack{\alpha\beta \\ \alpha\neq\beta}} \sum_{\substack{\gamma\delta \\ \gamma\neq\delta}} C_\beta^* C_\alpha C_\delta C_\gamma^* o_{\beta\alpha} o_{\delta\gamma}^* \tag{2.13}$$

$$= \sum_{\substack{\alpha\beta \\ \alpha\neq\beta}} |C_\alpha|^2 |C_\beta|^2 |o_{\beta\alpha}|^2 \tag{2.14}$$

$$\leq \sum_{\alpha\beta} |C_\alpha|^2 |C_\beta|^2 |o_{\beta\alpha}|^2 \tag{2.15}$$

$$= \mathrm{Tr}[\rho_{DE} \hat{o} \rho_{DE} \hat{o}^\dagger] \tag{2.16}$$

$$\leq ||\rho_{DE}\hat{o}|| \cdot ||\rho_{DE}\hat{o}^\dagger|| \tag{2.17}$$

$$= \sqrt{\mathrm{Tr}[\hat{o}^\dagger \rho_{DE} \rho_{DE} \hat{o}] \cdot \mathrm{Tr}[\hat{o} \rho_{DE} \rho_{DE} \hat{o}^\dagger]} \tag{2.18}$$

$$= \sqrt{\mathrm{Tr}[\hat{o}\hat{o}^\dagger \rho_{DE}^2] \cdot \mathrm{Tr}[\hat{o}^\dagger \hat{o} \rho_{DE}^2]} \tag{2.19}$$

$$\leq ||\hat{o}||^2 \mathrm{Tr}[\rho_{DE}^2] \tag{2.20}$$

$$= \frac{||\hat{o}||^2}{D_{\mathrm{eff}}}, \tag{2.21}$$

where we used the assumption (2.6) in (2.13), the Cauchy-Schwartz inequality for operators in (2.17), the cyclic symmetry of the trace in (2.19), and the relation for positive operators P and Q, $\mathrm{Tr}[PQ] \leq ||P||\mathrm{Tr}[Q]$ in (2.20).

By applying Chebyshev's inequality to Eq. (2.7), we immediately know for observables $\hat{o}$ with a physical range of spectrum that for arbitrary small ε, the fraction of the time during which $\langle\hat{o}\rangle$ differs more than ε from $\overline{\langle\hat{o}\rangle}$ decreases exponentially with respect to the system size V, provided that D_{eff} is rationally of order $e^{O(V)}$ [93]. The above illustrates the equilibration of closed macroscopic systems in terms of expectation values of observables. Therefore, we hereafter refer to the state ρ_d as the long-time steady state, or the state at equilibrium.

A few remarks are in order:

- Since a quantum state is written as Eq. (2.1), we can regard it as an assemble of D_c pieces of classical oscillators with frequencies E_α, where D_c is the number of eigenstates with nonzero C_α. Therefore, arbitrary dynamics in quantum mechanics takes an initial state arbitrarily close to itself after a finite time. In other words, it is (quasi)periodic [94]. This is called quantum recurrence. However, the recurrence time τ_{rec} is estimated as $\tau_{\mathrm{rec}} = e^{O(D_{\mathrm{eff}})}$ [3], and since we can as already mentioned, expect that D_{eff} grows exponentially with respect to the system size [93], it is generally extremely long. This implies that recurrence is irrelevant in observation of large enough systems.

- Although Eq. (2.7) assures that $\langle \hat{o} \rangle$ approximates Eq. (2.5) at most times, we cannot interpret it as fast relaxation towards the value Eq. (2.5) within the observation timescale. Indeed, the relaxation time is not discussed in the derivation so far. For instance, the inequality Eq. (2.7) does not exclude the known phenomenon of prethermalization [3], in which the system stays at a quasistationary state for a long time before reaching the true steady state. We stress that nevertheless we consider the long-time behavior and refer to the state ρ_d as the steady state.

- Although the assumption Eq. (2.6) is obviously not satisfied in noninteracting integrable systems, relaxation to a steady state is still seen in numerical simulations [87, 89] of such systems. It implies that while the theorem provides rigorous explanation for equilibration, the condition Eq. (2.6) does not need to be strictly satisfied for equilibration to occur.

Chapter 3

Strong/weak eigenstate thermalization hypothesis

In the previous section, the equilibration was explained in terms of expectation values of observables. One can see that thermalization can be explained if there is any mechanism of equalizing the value Eq. (2.5) with the value at thermal statistical ensembles. The ensemble can be any of the microcanonical ensemble, the Gibbs ensemble, and general grandcanonical ensembles owing to the equivalence between them. We will adopt the Gibbs ensemble in the following.

Hereafter we explain the eigenstate thermalization hypothesis (ETH) [18, 28, 29], and also a variant of the ETH, which is called the *weak ETH* [88]. The ETH is occasionally called the strong ETH, explicitly being distinguished from the weak ETH. The strong/(weak) ETH states that all/(almost all) eigenstates have thermal properties when we look at local properties. The strong ETH is a sufficient condition for thermalization, while the weak ETH is not [88].

The (strong) ETH is roughly a statement that the eigenstates inside an energy shell cannot be distinguished from the thermal state given by the Gibbs ensemble by looking at expectation values of spatially local observables. (Although few-body observables including nonlocal ones, instead of only local observables, are occasionally included in the statement, we restrict ourselves to spatially local observables throughout this thesis.) More concretely, the ETH is expressed as the following: when one considers an energy shell with half width Δ around an energy E, namely $S = S(E, \Delta) = (E-\Delta, E+\Delta)$, every eigenstate $|\alpha\rangle$ within the energy shell $E_\alpha \in S$ satisfies

$$\langle\alpha|\hat{o}|\alpha\rangle \approx \mathrm{Tr}[\hat{o}\rho_G], \tag{3.1}$$

for an arbitrary local observable $\hat{o}$, where ρ_G is the Gibbs ensemble $\rho_G = e^{-\beta\hat{H}}/\mathrm{Tr}[e^{-\beta\hat{H}}]$ with the inverse temperature β determined by the relation $\mathrm{Tr}[\hat{H}\rho_G] = E$. We take the half width Δ to be subextensive, i.e., macroscopically small and microscopically large enough. By macroscopically small we mean that $\Delta = o(V)$, with V the system size, e.g., $\Delta \propto L^{1/2}$. By microscopically large enough we mean that the number of eigenstates N_S in the shell is exponentially large in V, as in $N_S = e^{\mathcal{O}(V)}$. Assuming that the initial state is in an energy shell, which should be satisfied in realistic initial states, we see that if ETH is valid, then as to the value in Eq. (2.4),

$$\sum_\alpha |C_\alpha|^2 \langle\alpha|\hat{o}|\alpha\rangle \approx \sum_\alpha |C_\alpha|^2 \mathrm{Tr}[\hat{o}\rho_G] \tag{3.2}$$

$$= \mathrm{Tr}[\hat{o}\rho_G], \tag{3.3}$$

and thus the steady state cannot be distinguished from ρ_G by looking at the expectation value of local $\hat{o}$. Until now, there is no proof of ETH for any specific systems. The validity of ETH has been numerically checked for various nonintegrable models [47, 95], although a way of constructing counterexamples was found [96, 97]. (In [96, 97], it was discussed that the system may thermalize after a quench, despite the violation of ETH.)

Here, the important point is that Eq. (3.1) should be satisfied for *all* the eigenstates in the energy shell. It is called the weak ETH [88] when the fraction of eigenstates that do not satisfy Eq. (3.1) is negligibly small. Even in this case, the steady state may differ greatly from the thermal state ρ_G because the initial state may have an important weight on nonthermal energy eigenstates [88]. Indeed, the weak ETH can be proved for generic translationally invariant systems including integrable systems [88, 98, 99], although it is known that integrable systems generally do not thermalize [87–90]. The weak ETH is thus not enough to explain thermalization.

We note that the failure of description of the steady state in terms of usual statistical ensembles of the systems satisfying the weak ETH implies the following: realistic initial states such as those prepared by quench cannot, at least typically in the case of integrable systems, be considered to be a state that is taken from the energy shell with uniformly random measure. This is because it was discussed and proved under certain conditions in the context of typicality (see Sec. 1.1) that such randomly taken states are equivalent with the thermal state ρ_G with probability of unity in the thermodynamic limit [10, 21, 26, 27].

Chapter 4

Generalized Gibbs ensemble

As explained previously, it is at least typical for integrable systems that it does not relax to the usual Gibbs state [87–90]. It is suggested for integrable systems that its steady state is instead described by the so-called generalized Gibbs ensemble (GGE) [87]. The GGE is constructed by using many conserved quantities $\{Q_i\}$ of the system as in

$$\rho_{\mathrm{GGE}} = \frac{e^{-\sum_i \Lambda_i Q_i}}{\mathrm{Tr}\, e^{-\sum_i \Lambda_i Q_i}}, \tag{4.1}$$

where $\{\Lambda_i\}$ are the effective inverse-temperatures of $\{Q_i\}$, which are fixed by the initial state $|\psi_0\rangle$ according to the equations

$$\langle\psi_0|Q_i|\psi_0\rangle = \mathrm{Tr}\left[Q_i \rho_{\mathrm{GGE}}\right]. \tag{4.2}$$

Several numerical studies of various integrable systems have reported that the description of the steady state by the GGE seems to be consistent [2, 87, 89, 90]. By explicitly considering the time evolution of local observables, the validity of GGE has been proved for noninteracting integrable models with translation invariance under the assumption of the cluster-decomposition property of the initial state [100, 101]. However, the clarification of its generality is still in progress [90].

We note that there is an apparent ambiguity in the set of the conserved quantities that is to be included in $\{Q_i\}$ of Eq. (4.1). It has not been established in general how to prepare a sufficient, or preferably the minimum, set of conserved quantities appropriate for Eq. (4.1) to describe the steady state correctly, especially for interacting integrable systems. Nevertheless, as for noninteracting systems, the set of all the mode occupations (shown below for a simple case) is considered as a sufficient set [87, 100, 101].

4.1 Local conserved quantities

The form of GGE is not unique, because the set of conserved quantities can be linearly transformed to a different set [90]. Let us explain this for the simple case of a fermionic tight-binding model given by

$$H = -J \sum_x c_x^\dagger c_{x+1} + c_{x+1}^\dagger c_x - h \sum_x c_x^\dagger c_x, \tag{4.3}$$

where $\{c_x, c_y^\dagger\} = \delta_{x,y}$. The Fourier transformation $f_p^\dagger = (1/\sqrt{L}) \sum_{x=1}^{L} c_x^\dagger e^{-ipx}$ diagonalizes the Hamiltonian as

$$H = \sum_p \left[-2J \cos(p) - h\right] f_p^\dagger f_p. \tag{4.4}$$

Each of the mode occupation operators $\{f_p^\dagger f_p\}$ commutes with the Hamiltonian. Thus we can construct the GGE as

$$\rho_{\mathrm{GGE}}^{(1)} = \frac{e^{-\sum_p \lambda_p f_p^\dagger f_p}}{\mathrm{Tr}\left[e^{-\sum_p \lambda_p f_p^\dagger f_p}\right]}. \tag{4.5}$$

Now the conserved quantities $\{f_p^\dagger f_p\}$ taken into account are not spatially local, nor macroscopic.

We can construct another set of conserved quantities by a linear combination of $\{f_p^\dagger f_p\}$ as

$$\begin{cases} \mathcal{Q}_n^{(+)} = 2J \sum_p \cos(np) f_p^\dagger f_p = J \sum_x c_x^\dagger c_{x+n} + c_{x+n}^\dagger c_x, \\ \mathcal{Q}_n^{(-)} = 2J \sum_p \sin(np) f_p^\dagger f_p = iJ \sum_x c_x^\dagger c_{x+n} - c_{x+n}^\dagger c_x. \end{cases} \tag{4.6}$$

These conserved quantities $\mathcal{Q}_n^{(\pm)}$ are spatially local. The GGE for this set of conserved quantities is given by

$$\rho_{\mathrm{GGE}}^{(2)} = \frac{\exp\left[-\sum_n \left(\Lambda_n^{(+)} \mathcal{Q}_n^{(+)} + \Lambda_n^{(-)} \mathcal{Q}_n^{(-)}\right)\right]}{\mathrm{Tr}\left(\exp\left[-\sum_n \left(\Lambda_n^{(+)} \mathcal{Q}_n^{(+)} + \Lambda_n^{(-)} \mathcal{Q}_n^{(-)}\right)\right]\right)}. \tag{4.7}$$

The two sets of conserved quantities are linearly related. Therefore, the two forms of GGEs (4.5) and (4.7) constructed for a common initial state $|\psi_0\rangle$ as in (4.2) must be equal to each other.

4.2 Importance of locality of the conserved quantities

Constructing a set of conserved quantities in terms of local ones is critical because it has been recognized that of all such conserved quantities, it is the local ones that play important roles in the local properties of the steady state of integrable systems [90,102]. In [102], this was made evident by considering a truncation of the local conserved quantities. Here we explain this for the transverse Ising model, following Ref. [102], although we omit specific calculations. The Hamiltonian is given by

$$H = -J\sum_j \left(\sigma_j^x\sigma_{j+1}^x + h\sigma_j^z\right), \tag{4.8}$$

for which we demand the periodic boundary condition $\sigma_{L+1}^\alpha = \sigma_1^\alpha$. Using the Jordan-Wigner transformation [103] followed by the Bogoliubov transformation (see Sec. 5.1.2), the Hamiltonian is diagonalized in terms of the mode occupation operators of a new set of fermions η_p as

$$H = \sum_p \tilde{\varepsilon}_p \eta_p^\dagger \eta_p + \text{const}, \tag{4.9}$$

where $\tilde{\varepsilon}_p = 2J\sqrt{1+h^2-2h\cos(p)}$ is the single-particle energy. The local conserved quantities for this system are given by (see Sec. 5.1.2)

$$\begin{cases} \mathcal{Q}_n^{(+)} = \sum_p \cos(np)\tilde{\varepsilon}_p\eta_p^\dagger\eta_p, \\ \mathcal{Q}_n^{(-)} = -2J\sum_p \sin(np)\eta_p^\dagger\eta_p. \end{cases} \tag{4.10}$$

The GGE is again given by the form

$$\rho_{\text{GGE}} = \frac{\exp\left[-\sum_n\left(\Lambda_n^{(+)}\mathcal{Q}_n^{(+)} + \Lambda_n^{(-)}\mathcal{Q}_n^{(-)}\right)\right]}{\text{Tr}\left(\exp\left[-\sum_n\left(\Lambda_n^{(+)}\mathcal{Q}_n^{(+)} + \Lambda_n^{(-)}\mathcal{Q}_n^{(-)}\right)\right]\right)} \tag{4.11}$$

with $\mathcal{Q}_n^{(\pm)}$ defined by Eq. (4.10). The truncated GGE introduced in Ref. [102] is defined as

$$\rho_{\text{tGGE}}^{(y)} = \frac{1}{\mathcal{Z}^{(y)}}\exp\left[-\sum_n^y\left(\Lambda_n^{(+,y)}\mathcal{Q}_n^{(+)} + \Lambda_n^{(-,y)}\mathcal{Q}_n^{(-)}\right)\right], \tag{4.12}$$

where $\mathcal{Z}^{(y)}$ is the normalization factor.

Reference [102] considered the trace distance

$$\mathcal{D}(\rho,\rho') = \frac{\sqrt{\text{Tr}(\rho^2+\rho'^2-2\rho\rho')}}{\sqrt{\text{Tr}(\rho^2)+\text{Tr}(\rho'^2)}} \tag{4.13}$$

between the reduced matrices of the subsystems of the GGE ρ_{GGE} and the truncated GGEs $\rho^{(y)}_{\mathrm{tGGE}}$. The reduced matrix of a subsystem with l spins at site $j = 1, \ldots, l$ can be expressed as

$$\rho_{\{1,\ldots,l\}} = \frac{1}{2^l} \sum_{\{\alpha\}_l} \mathrm{Tr}[\rho \sigma_1^{\alpha_1} \ldots \sigma_l^{\alpha_l}] \sigma_1^{\alpha_1} \ldots \sigma_l^{\alpha_l}, \tag{4.14}$$

where $\alpha_j = 0, x, y, z$. The trace distance $\mathcal{D}(\rho_{\mathrm{GGE}\{1,\ldots,l\}}, \rho^{(y)}_{\mathrm{tGGE}\{1,\ldots,l\}})$ was numerically calculated for a quench from $h = 1.2$ to $h = 3$ for the infinite transverse Ising chain. They found [102] that $\mathcal{D}(\rho_{\mathrm{GGE}\{1,\ldots,l\}}, \rho^{(y)}_{\mathrm{tGGE}\{1,\ldots,l\}})$ decreases monotonically for y, and that the decreasing becomes rapid for $y > l$, namely exponentially. This shows that the local conserved quantities are critical for local properties of the steady state. The authors of [102] expected that this is a general feature in integrable systems.

4.3 GGE for interacting integrable systems

For interacting integrable systems, searching the form of an adequate GGE appears to be a much more subtle problem than in the case of noninteracting integrable systems. Up to now, the interacting integrable system most understood in this context is the spin-1/2 XXZ model, whose Hamiltonian is

$$H = \frac{J}{4} \sum_{j=1}^{L} \left[\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + \Delta(\sigma_j^z \sigma_{j+1}^z - 1) \right], \tag{4.15}$$

where $J > 0$ and we consider $\Delta \geq 1$. This system is solved by the Bethe Ansatz [85]. In [104, 105], a GGE was constructed by a set of local conserved quantities $\{H^{(n)}\}$, where $H^{(1)}$ is the Hamiltonian and $[H^{(n)}, H^{(m)}] = 0$. However, in [106, 107], it was revealed that thus constructed GGE fails to correctly give identical predictions of the properties of the steady state, to which are calculated by the Quench Action method [108, 109]. Although we do not go into the details, the Quench Action is a method that enables one to calculate the expectation value of observables in the steady state realized after a quench, in a way similar to the thermodynamic Bethe Ansatz [110]. It is formulated within the thermodynamic limit, under the assumption that a kind of course-graining procedure which is necessary in defining an effective action, called the "Quench Action," is valid. In Ref. [111], this problem was resolved by considering the so-called quasilocal conserved quantities, which were discovered for the isotropic ($\Delta = 1$) XXZ model in Ref. [112] and later generalized for $\Delta \geq 1$ in Ref. [111]. Quasilocal conserved quantities are not local in the sense that they cannot be written as a sum of operators that are supported by a finite region of a system. Instead they are defined as operators Q satisfying the following two conditions [112]: (i) their Hilbert-Schmidt norms scale linearly with system size V as in $||Q||_{\mathrm{HS}} := (Q, Q) \propto V$, where $(A, A) \equiv \mathrm{Tr}(A^\dagger A)$ and (ii) for any locally supported operators b, their overlap (b,Q) is asymptotically independent of V in the limit $V\to\infty$. Reference [111] defined a two-parameter family of quasilocal conserved quantities $\{H_n^{(s/2)}\}_{s,n=1}^{\infty}$, where $[H_n^{(s/2)},H_m^{(s'/2)}]=0$ and $\{H_n^{(1/2)}\}_{n=1}^{\infty}$ are the local conserved quantites considered in Ref. [104, 105]. Reference [111] used it to construct a GGE in the form

$$\rho_{\rm GGE}=\frac{1}{\mathcal{Z}}\exp\left[-\sum_{n,s=1}^{\infty}\Lambda_{n,s}H_n^{(s/2)}\right], \tag{4.16}$$

where again $\mathcal{Z}$ is the normalization constant and $\Lambda_{n,s}$ are determined by the initial state. It was shown analytically [111] that the GGE in Eq. (4.16) gives an identical prediction of the properties of the steady state to that calculated by the Quench Action method. The authors of Ref. [111] also questioned whether the prediction of the steady state still persists after the truncation of conserved quantities (see Sec. 4.2). They numerically compared the expectation value of the spin correlation $\langle\sigma_1^z\sigma_3^z\rangle$, on one side calculated by the Quench Action method, and on the other side by the GGE's where the higher families of the quasilocal conserved quantities are truncated, as in

$$\rho^{(s_c)}=\frac{1}{\mathcal{Z}^{(s_c)}}\exp\left[-\sum_{s=1}^{s_c}\sum_{n=1}^{\infty}\Lambda_{n,s}H_n^{(s/2)}\right]. \tag{4.17}$$

They calculated for $s_c=1/2,\ 1,\ 3/2,\ 2$ and for several values of anisotropy in the range $1<\Delta<1.05$ and found that for all the values of Δ under study, the correlation rapidly converges to the exact value obtained by the Quench Action methods as they included higher families of the quasilocal conserved quantities. (See Fig. 1 in Ref. [111] for details.)

In the following sections, we only consider noninteracting integrable systems. The generalization to interacting integrable systems of the discussions to appear in the following is an issue of future perspective.

Chapter 5

Generalization of the strong ETH

A particular set of questions on GGE naturally arises in accordance with the ETH explained in Chapter 3. That is, can one construct any generalized version of the ETH as a mechanism that explains the equilibration to the GGE, just as thermalization in nonintegrable systems is explained by the ETH? If so, can we remove the assumption of the cluster-decomposition property [100, 101] for the initial state in deriving the equilibration to the GGE? The removal of this assumption is important in considering a spin system that can be mapped to a quadratic fermion Hamiltonian (e.g., the transverse-field Ising model) because it is not obvious whether a physically realistic initial state, which satisfies the cluster-decomposition property *with respect to the spin operators*, satisfies it *with respect to the fermion operators* too [113].

In Ref. [89], a generalization of the ETH has been proposed. Their generalized ETH has been numerically verified [89] and also proved for various local operators in the translationally invariant transverse-field Ising model [114], but *only in the weak sense*. It has not been clarified yet whether it is valid in the strong sense. Although the concept of the generalized ETH helps us to understand the validity of the GGE [89, 114], the weak generalized ETH does not ensure in itself the relaxation to a GGE in an integrable system. It is therefore desirable to formulate the generalized ETH that is valid in the strong sense.

In this chapter, by constructing a generalized shell that is specified by a set of macroscopic conserved quantities, we reformulate the generalized ETH and analytically prove that our generalized ETH proposed is valid *in the strong sense* in integrable models of the quadratic form with translation invariance. We show that our strong generalized ETH ensures the relaxation to a GGE for initial states that have subextensive fluctuations of macroscopic local conserved quantities. The condition of subextensive fluctuations of macroscopic local conserved quantities is much weaker than the condition of the cluster-decomposition property; the latter implies the former, but the former does not imply the latter (we will come back to this point in Sec. 5.4). We manage to remove the assumption

	Hilbert subspace	steady state	validity
strong ETH [18, 47, 88, 95–97, 115]	energy shell	Gibbs ensemble	nonintegrable: valid but with counterexamples. integrable: invalid.
strong generalized ETH (present study)	shell defined by many macroscopic conserved quantities	generalized Gibbs ensemble	translationally invariant noninteracting integrable: valid.

Table 5.1: A comparison between the strong ETH [18, 47, 88, 95–97, 115] and our strong generalized ETH. While the usual strong ETH is discussed for states in the energy shell, in the formulation of our strong generalized ETH, we consider a generalized shell, which is defined as a Hilbert subspace specified by a set of macroscopic conserved quantities. The strong ETH and our strong generalized ETH are sufficient conditions for relaxation to the steady state described by the Gibbs ensemble and the generalized Gibbs ensemble, respectively. In the column indicated "validity," we explain the current understanding on the validity of the two concepts. As for the strong ETH, in nonintegrable systems, its validity has been numerically confirmed [47,95], although there exist some counterexamples [96,97]. In integrable systems, numerical demonstrations and analytical calculations show that the strong ETH does not hold [18, 88, 95, 115]. As for our strong generalized ETH, we analytically prove in this thesis its validity in translationally invariant noninteracting integrable systems.

of the cluster-decomposition property here, in which sense our result is beyond the previous rigorous results [100, 101]. In Table 5.1 we show for help of understanding a comparison between the strong ETH and our strong generalized ETH.

This chapter is organized as follows. In section 5.1, we explain the model considered and introduce the generalization of the strong ETH to integrable systems. In 5.2.2, we discuss the relation to the generalized ETH suggested in a previous work [89]. In section 5.3 we provide a proof of the strong generalized ETH.

5.1 Model and setup

We consider a quadratic fermion system described by the translationally invariant Hamiltonian

$$H = \sum_{x,y=1}^{L} \left(c_x^\dagger A_{x-y} c_y + c_x^\dagger B_{x-y} c_y^\dagger + c_x B_{y-x}^* c_y \right), \tag{5.1}$$

under the periodic boundary condition [1]. (The coefficients A_l and B_l are complex values with one variable l. The fact that they depend only on the difference $x - y$ of sites x

[1] In the case of the anti-periodic boundary condition, where the quadratic terms acquire an extra minus-sign when the two annihilation or creation operators are involved across the boundary (e.g., terms including A_1 is $c_2^\dagger A_1 c_1 + c_3^\dagger A_1 c_2 + \cdots + c_L^\dagger A_1 c_{L-1} - c_1^\dagger A_1 c_L$), the specific wave numbers which constitutes the quantum labels change, but this does not essentially affect our analysis.

and y implies the translation invariance of the Hamiltonian.) The coefficients A_l satisfies $A_l = A^*_{-l}$ because $H = H^\dagger$. We assume the locality of the Hamiltonian, i.e., $A_l = B_l = 0$ for $|l|_P > r_H$ with a finite range $r_H > 0$, where $|l|_P := \min\{|l|, L-|l|\}$ denotes the distance l under the periodic boundary condition. This form of Hamiltonian includes, for example, a fermionic system with on-site potential and nearest-neighbor hopping terms. The XY model, a hard-core boson system, and the transverse-field Ising model can also be mapped to this form using the Jordan-Wigner transformation.

5.1.1 Models with $B_{x-y} = 0$

We first consider the case of $B_l = 0$, for which the total particle number is conserved. This system can be diagonalized by the Fourier transform as

$$H = \sum_p \varepsilon_p f_p^\dagger f_p, \tag{5.2}$$

where $f_p^\dagger = (1/\sqrt{L}) \sum_{x=1}^L c_x^\dagger e^{-ipx}$ and $\varepsilon_p = \sum_{x=1}^L A_x e^{ipx}$. The summation over $p = 2\pi m/L$ is taken over integers m with $-(L-1)/2 \leq m \leq (L-1)/2$, where we consider the case of odd L throughout the paper, although this restriction is not essential.

The occupation-number operator of each of the L eigenmodes $\{f_p^\dagger f_p\}$ is a conserved quantity. Although the operators $\{f_p^\dagger f_p\}$ are not spatially local, we can construct macroscopic local conserved quantities out of them as

$$\begin{cases} \mathcal{Q}_n^{(+)} = \sum_p \cos(np) f_p^\dagger f_p, & n = 0, 1, \ldots, \dfrac{L-1}{2}, \\ \mathcal{Q}_n^{(-)} = \sum_p \sin(np) f_p^\dagger f_p, & n = 1, \ldots, \dfrac{L-1}{2}; \end{cases} \tag{5.3}$$

see Ref. [90]. We then define $\mathcal{Q}_{-n}^{(+)} = \mathcal{Q}_n^{(+)}$, $\mathcal{Q}_{-n}^{(-)} = -\mathcal{Q}_n^{(-)}$, and $\mathcal{Q}_0^{(-)} = 0$. Note that $\mathcal{Q}_0^{(+)}$ coincides with the total particle number:

$$\mathcal{Q}_0^{(+)} = \sum_p f_p^\dagger f_p = \hat{N}. \tag{5.4}$$

We denote an eigenvalue of $\mathcal{Q}_n^{(\pm)}$ for the Fock eigenstates by $Q_n^{(\pm)}$.

5.1.2 Models with $B_{x-y} \neq 0$

When $B_l \neq 0$, the Bogoliubov transformation following the Fourier transformation diagonalizes the Hamiltonian as

$$H = \sum_p \tilde{\varepsilon}_p \eta_p^\dagger \eta_p + \text{const.}, \tag{5.5}$$

where $\tilde{\varepsilon}_p$ and $\eta_p^\dagger$ are given by $a_p := \sum_{x=1}^{L} A_x e^{ipx}$ and $b_p := 2i\sum_{x=1}^{L} B_x \sin(px)$ as

$$\tilde{\varepsilon}_p = \frac{a_p - a_{-p} + \sqrt{(a_p + a_{-p})^2 + 4|b_p|^2}}{2}, \tag{5.6}$$

$$\eta_p^\dagger = s(p) f_p^\dagger + t(p) f_{-p}, \tag{5.7}$$

with the functions $s(p)$ and $t(p)$ defined as

$$s(p) = \frac{|b_p|}{\sqrt{|b_p|^2 + (\tilde{\varepsilon}_p - a_p)^2}}, \tag{5.8}$$

$$t(p) = \frac{|b_p|}{b_p} \frac{\tilde{\varepsilon}_p - a_p}{\sqrt{|b_p|^2 + (\tilde{\varepsilon}_p - a_p)^2}}. \tag{5.9}$$

Macroscopic local conserved quantities in this case are given by

$$\begin{cases} \mathcal{Q}_n^{(+)} = \dfrac{1}{2} \displaystyle\sum_p \cos(np)(\tilde{\varepsilon}_p + \tilde{\varepsilon}_{-p}) \eta_p^\dagger \eta_p, \\ \mathcal{Q}_n^{(-)} = \displaystyle\sum_p \sin(np) \eta_p^\dagger \eta_p, \end{cases} \tag{5.10}$$

where we use the same notations as in Eq. (5.3), but there will be no confusion.

The locality of $\mathcal{Q}_n^{(+)}$ in Eq. (5.10) is proved as follows. First, we divide it into two parts as follows:

$$\mathcal{Q}_n^{(+)} = \sum_p \tilde{\varepsilon}_p \cos(np) \eta_p^\dagger \eta_p + \sum_p \frac{\tilde{\varepsilon}_p - \tilde{\varepsilon}_{-p}}{2} \cos(np) \eta_p^\dagger \eta_p. \tag{5.11}$$

It is known and explicitly confirmed that the first term of Eq. (5.11) is local [102]. As for the second term, we notice that $\tilde{\varepsilon}_p - \tilde{\varepsilon}_{-p} = a_p - a_{-p}$ is written as a finite sum $\sum_{x=-r_H}^{r_H} A_x(e^{ipx} - e^{-ipx})$ because of the fact that $\hat{H}$ is a local operator with the maximum range r_H. Therefore, the second term of Eq. (5.11) is written as a linear combination of $\{\mathcal{Q}_m^{(-)}\}$ with $m \le n + r_H$, which is a local operator. Thus, for any fixed n, both the first and the second terms of Eq. (5.10) are local in the thermodynamic limit.

In terms of these local conserved quantities, the GGE is given as the density matrix

$$\rho_{\mathrm{GGE}} = \frac{e^{-\sum_{n=0}^{(L-1)/2} \left(\Lambda_n^{(+)} \mathcal{Q}_n^{(+)} + \Lambda_n^{(-)} \mathcal{Q}_n^{(-)} \right)}}{Z_{\mathrm{GGE}}}, \tag{5.12}$$

where Z_{GGE} is the normalization constant. The parameters $\Lambda_p^{(\pm)}$ are determined from the initial state $|\psi(0)\rangle$ by the condition that $\langle \psi(0) | \mathcal{Q}_n^{(\pm)} | \psi(0) \rangle = \mathrm{Tr}[\mathcal{Q}_n^{(\pm)} \rho_{\mathrm{GGE}}]$.

5.2 Formulation of the generalized ETH

5.2.1 Formulation

In order to formulate our generalized ETH, we first define a Hilbert subspace called an n_c-shell with the notation $\mathcal{S}_{n_c}$. Let us denote the set of the simultaneous eigenstates of $\{\mathcal{Q}_n^{(\pm)}\}$ by $\mathcal{E}$. An n_c-shell is then defined as a Hilbert subspace spanned by all the eigenstates in $\mathcal{E}$ with the eigenvalues located around the center $\{\bar{Q}_n^{(\pm)}\}_{n=1}^{n_c}$:

$$\begin{aligned}\mathcal{S}_{n_c} :=& \mathrm{Span}\Big\{|\alpha\rangle \in \mathcal{E} : \text{ for all } 0 \leq n \leq n_c, \\ & Q_n^{(\pm)} \in [\bar{Q}_n^{(\pm)} - \Delta_n^{(\pm)}, \bar{Q}_n^{(\pm)} + \Delta_n^{(\pm)}]\Big\}. \end{aligned} \tag{5.13}$$

Here, the half width of the shell $\Delta_n^{(\pm)}$ is arbitrary as long as it is subextensive, i.e., macroscopically small but microscopically large. By macroscopically small, we mean that $\Delta_n^{(\pm)} = o(L)$. By microscopically large, we mean that the number of eigenstates $N_{\mathcal{S}_{n_c}}$ in $\mathcal{S}_{n_c}$, as well as the number of eigenstates $N_n^{(\pm)}$ in each of the region $Q_n^{(\pm)} \in [\bar{Q}_n^{(\pm)} - \Delta_n^{(\pm)}, \bar{Q}_n^{(\pm)} + \Delta_n^{(\pm)}]$, for each n with $n \leq n_c$, are all exponentially large in L, as in $N_{\mathcal{S}_{n_c}} = e^{\mathcal{O}(L)}$ and $N_n^{(\pm)} = e^{\mathcal{O}(L)}$. For example, we can choose $\Delta_n^{(\pm)} \propto L^{1/2}$. Note that n runs up to $n_c \leq (L-1)/2$. The n_c-shell can be regarded as a generalization of the usual energy shell in the microcanonical ensemble.

The n_c-shell implies that conserved quantities with n up to n_c are taken into account. For example, the 3-shell is a generalized shell where $Q_0^{(+)}$, $Q_1^{(\pm)}$, $Q_2^{(\pm)}$, and $Q_3^{(\pm)}$ are taken into account. We note beforehand that in the case of $B_{x-y} = 0$, we shall show in Sec. 5.3.1 that a truncated GGE with only $Q_0^{(+)}$, $Q_1^{(\pm)}$, $Q_2^{(\pm)}$, and $Q_3^{(\pm)}$ taken into account correctly gives expectation values of observables with maximum range 3, of the steady state.

Now we formulate the strong generalized ETH. It states that all the energy eigenstates in $\mathcal{S}_{n_c}$ are locally indistinguishable from each other in the limit of $n_c \to \infty$ taken after the thermodynamic limit $L \to \infty$. For convenience, we also say that a local observable $\hat{o}$ satisfies the n_c-ETH when $\langle\alpha|\hat{o}|\alpha\rangle = \langle\alpha'|\hat{o}|\alpha'\rangle$ for any pair of eigenstates $|\alpha\rangle, |\alpha'\rangle \in \mathcal{S}_{n_c}$ in the thermodynamic limit.

5.2.2 Relation with a different generalization of ETH in a previous work

Besides our formulation of the generalized strong ETH explained above, another generalization of ETH has been proposed in the previous work [89], stating that energy eigenstates with similar distributions of the mode occupation number look similar with respect to local observables. They considered the case of noninteracting integrable models where the total particle number is conserved. Below we explain the relation between our generalized ETH based on the n_c-shell and the generalized ETH based on the mode occupation number distributions, which is a simplified version of the one originally proposed in Ref. [89].

For simplicity, we consider the case in which the total particle number is conserved with $B_l = 0$. Then, each energy eigenstate $|\alpha\rangle$ consists of N occupied levels $\{p_1^\alpha, p_2^\alpha, \ldots, p_N^\alpha\}$, where $p_i^\alpha = 2\pi n_i^\alpha / L$ with integers $\{n_i^\alpha\}_{i=1}^N$ satisfying $-\pi \leq p_1^\alpha < p_2^\alpha < \cdots < p_N^\alpha < \pi$. In short, $\langle\alpha|f_p^\dagger f_p|\alpha\rangle = 1$ if and only if $p \in \{p_1^\alpha, p_2^\alpha, \ldots, p_N^\alpha\}$. Let us say that two eigenstates $|\alpha\rangle$ and $|\alpha'\rangle$ have 'similar' distributions of the mode occupation number if and only if

$$\delta(\alpha, \alpha') = \left[\frac{1}{N}\sum_{i=1}^{N}\left(p_i^\alpha - p_i^{\alpha'}\right)^2\right]^{1/2} \tag{5.14}$$

is smaller than a threshold ϵ, which can be set to zero in the thermodynamic limit. The generalized ETH formulated in Ref. [89] essentially states that two eigenstates with similar distributions of the mode occupation number are locally indistinguishable. Now we begin the explanation of its relation with our generalized ETH. Let us consider the difference between macroscopic conserved quantities in the states $|\alpha\rangle$ and $|\alpha'\rangle$:

$$\delta q_n^{(\pm)} := \frac{1}{L}\left|\langle\alpha|\mathcal{Q}_n^{(\pm)}|\alpha\rangle - \langle\alpha'|\mathcal{Q}_n^{(\pm)}|\alpha'\rangle\right|. \tag{5.15}$$

If $|\delta q_n^{(\pm)}| \leq 2\Delta_n^{(\pm)}/L$ for all $n \leq n_c$, the two eigenstates $|\alpha\rangle$ and $|\alpha'\rangle$ belong to the same n_c-shell under a suitable choice of the center of the shell $\{\bar{Q}_n^{(\pm)}\}_{n=1}^{n_c}$. By using p_i^α, we can rewrite $\delta q_n^{(+)}$ as

$$\begin{aligned}\delta q_n^{(+)} &= \frac{1}{L}\left|\sum_{i=1}^{N}[\cos(np_i^\alpha) - \cos(np_i^{\alpha'})]\right| \\ &\leq \frac{1}{L}\sum_{i=1}^{N}\left|\cos(np_i^\alpha) - \cos(np_i^{\alpha'})\right|.\end{aligned} \tag{5.16}$$

By using $|\cos\theta - \cos\phi| \leq |\theta - \phi|$, we obtain

$$\begin{aligned}\delta q_n^{(+)} &\leq \frac{n}{L}\sum_{i=1}^{N}|p_i^\alpha - p_i^{\alpha'}| \\ &\leq n\rho\delta(\alpha, \alpha'),\end{aligned} \tag{5.17}$$

where $\rho = N/L$ and we have used $\delta(\alpha, \alpha') \geq (1/N)\sum_{i=1}^{N}|p_i^\alpha - p_i^{\alpha'}|$. Similarly, $\delta q_n^{(-)} \leq n\rho\delta(\alpha, \alpha')$ holds.

From these inequalities, we can immediately conclude that two eigenstates $|\alpha\rangle$ and $|\alpha'\rangle$ belong to the same n_c-shell under a suitable choice of $\{\bar{Q}_n^{(\pm)}\}_{n=1}^{n_c}$ as long as $\delta(\alpha, \alpha') \leq 2\Delta_n^{(\pm)}/(n_c N)$. Since $\Delta_n^{(\pm)}$ is chosen so that $\Delta_n^{(\pm)}/N \to 0$ in the thermodynamic limit, this result implies that two eigenstates $|\alpha\rangle$ and $|\alpha'\rangle$ with similar distributions of the mode occupation number belong to the same n_c-shell. This implies that if the generalized ETH based on the n_c-shell holds in the strong sense, then the generalized ETH based on the similarity of the distributions of the mode occupation number also holds in the strong sense. (It should be noted that the converse is not true in general.) Thus the proof of the strong generalized ETH based on the n_c-shell complements the numerical result in Ref. [89], in which the generalized ETH based on the mode occupation number distribution has been confirmed only in the weak sense.

5.3 Proof of the strong generalized ETH

We consider local observables $\hat{o}$ which consist of fermionic operators $\{c^\dagger, c\}$ with the maximum range r. For example,

$$\hat{o} = \frac{1}{L}\sum_{j=1}^{L}\left(c_{j+2}^\dagger c_{j+2} c_j^\dagger c_j + c_{j+1}^\dagger c_j + c_j^\dagger c_{j+1}\right) \tag{5.18}$$

is the case of $r = 2$. As a shorthand notation, we write $\langle \hat{o} \rangle := \langle \alpha|\hat{o}|\alpha\rangle$ for a fixed eigenstate $|\alpha\rangle$.

5.3.1 Models with $B_{x-y} = 0$

We first consider the case $B_l = 0$, in which the total particle number is conserved. In this case, the diagonalized Hamiltonian is given by Eq. (5.2) and macroscopic conserved quantities are given by Eq. (5.3). We shall prove that the eigenstate expectation value of a local observable can be written as a smooth function of the eigenvalues $\{Q_m^{(\pm)}/L\}$ of the constructed conserved quantities with $m \le r$. In other words, any local observable with the maximum range r satisfies the r-ETH.

By virtue of Wick's theorem, the eigenstate expectation value $\langle \hat{o} \rangle$ of any local observable $\hat{o}$ with the maximum range r can be decomposed into products of two-point functions of the form $\langle c_x^\dagger c_y \rangle$ with $|x-y|_P \le r$. Note that although Wick's theorem is usually applied to the vacuum state, it can be applied to individual eigenstates too in the present systems because the eigenstates can be expressed as a vacuum state by redefining the particles and holes for each mode (See Ref. [116]). More precisely, if we denote by X_i a linear superposition of $\{c_x, c_x^\dagger\}$,

$$\begin{aligned}&\langle X_1 X_2 \dots X_{2n}\rangle \\ &= \sum (-1)^P \langle X_{i_1} X_{j_1}\rangle \langle X_{i_2} X_{j_2}\rangle \dots \langle X_{i_n} X_{j_n}\rangle,\end{aligned} \tag{5.19}$$

where the sum is over all partitions of $1, 2, \dots 2n$ into pairs $\{(i_1, j_1), (i_2, j_2), \dots, (i_n, j_n)\}$ with $i_1 < j_1$, $i_2 < j_2, \dots i_n < j_n$, and P is the parity of the permutation $(1, 2, \dots, 2n) \to$

$(i_1, j_1, i_2, j_2, \ldots, i_n, j_n)$ [116]. It should be noted that Eq. (5.19) also holds even when $B_l \neq 0$ because the Bogoliubov fermion operators η_p and $\eta_p^\dagger$ can be written as a linear superposition of $\{c_x, c_x^\dagger\}$.

We can express the two-point function in terms of the conserved quantities in Eq. (5.3) as in

$$\begin{aligned}\langle c_x^\dagger c_y \rangle &= \frac{1}{L} \sum_p e^{ip(x-y)} \langle f_p^\dagger f_p \rangle \\ &= \frac{1}{L}(Q_{x-y}^{(+)} + iQ_{x-y}^{(-)}).\end{aligned} \tag{5.20}$$

Therefore, $\langle \hat{o} \rangle$ is generally a smooth function of $\{Q_m^{(\pm)}/L\}$ with $m \leq r$.

This immediately leads to the validity of the strong generalized ETH. Moreover, any local operator with the maximum range $r \leq n_c$ satisfies the n_c-ETH. Therefore, as far as we consider local operators with a fixed maximum range r, the steady state is described by the microcanonical ensemble within the n_c-shell, which is in the thermodynamic limit equivalent to the *truncated* GGE,

$$\rho_{\mathrm{GGE}}^{(n_c)} := \frac{\exp\left[-\sum_{n=0}^{n_c}\left(\Lambda_n^{(+)}\mathcal{Q}_n^{(+)} + \Lambda_n^{(-)}\mathcal{Q}_n^{(-)}\right)\right]}{Z_{\mathrm{GGE}}^{(n_c)}}, \tag{5.21}$$

for an arbitrary $n_c \geq r$, where $Z_{\mathrm{GGE}}^{(n_c)}$ is the normalization factor. In the limit of $n_c \to \infty$ after the thermodynamic limit, the GGE reproduces expectation values of arbitrary local operators in the steady state.

5.3.2 Models with $B_{x-y} \neq 0$

Next, we consider free fermion models in which the total particle number is not conserved ($B_l \neq 0$). The eigenstate expectation value of a local operator is again decomposed into the products of two-point functions. Relevant two-point functions are $\langle c_x^\dagger c_y \rangle$ and $\langle c_x^\dagger c_y^\dagger \rangle$ with $|x-y|_P \leq r$, the latter of which appears because $B_{x-y} \neq 0$. By expressing these two-point functions using the mode occupation numbers $\eta_p^\dagger \eta_p$, we have

$$\begin{aligned}\langle c_x^\dagger c_y \rangle =& \frac{1}{L} \sum_p \cos[p(x-y)] \left(s(p)^2 - |t(p)|^2\right) \langle \eta_p^\dagger \eta_p \rangle \\ &+ \frac{i}{L} \sum_p \sin[p(x-y)] \langle \eta_p^\dagger \eta_p \rangle + \mathrm{const.},\end{aligned} \tag{5.22}$$

and

$$\langle c_x^\dagger c_y^\dagger \rangle = \frac{2i}{L} \sum_p \sin[p(x-y)] s(p) t(p) \langle \eta_p^\dagger \eta_p \rangle + \mathrm{const.} \tag{5.23}$$

By performing the Fourier series expansion, we can express $\langle c_x^\dagger c_y\rangle$ and $\langle c_x^\dagger c_y^\dagger\rangle$ as

$$\langle c_x^\dagger c_y\rangle = \frac{v_0}{L} Q_{x-y}^{(+)} + \frac{1}{L}\sum_{n=1}^{(L-1)/2} v_n \left(Q_{x-y+n}^{(+)} + Q_{x-y-n}^{(+)} \right) + \frac{i}{L} Q_{x-y}^{(-)} + \text{const.}, \tag{5.24}$$

and

$$\langle c_x^\dagger c_y^\dagger\rangle = -\frac{i}{L}\sum_{n=1}^{(L-1)/2} w_n \left(Q_{x-y+n}^{(+)} - Q_{x-y-n}^{(+)} \right) + \text{const.} \tag{5.25}$$

Here, v_n in Eq. (5.24) and w_n in Eq. (5.25) are the Fourier coefficients of

$$\frac{2}{\tilde{\varepsilon}(p) + \tilde{\varepsilon}(-p)} \left(s(p)^2 - |t(p)|^2 \right) \tag{5.26}$$

and

$$\frac{4i}{\tilde{\varepsilon}(p) + \tilde{\varepsilon}(-p)} s(p) t(p), \tag{5.27}$$

respectively, where the Fourier coefficient of $\phi(p)$ is defined by $\phi_n = (1/L)\sum_p \phi(p) e^{-ipn}$. It is noted that the relations $v_n = v_{-n}$ and $w_n = -w_{-n}$, which follow from the parity of the functions (5.26) and (5.27), are used in deriving Eqs. (5.24) and (5.25). According to the Riemann-Lebesgue lemma, v_n and w_n tend to zero in the limit of $|n| \to \infty$ taken after the thermodynamic limit [2]. Therefore, we can approximately truncate the summations over n in Eqs. (5.24) and (5.25) at a sufficiently large n^*, e.g.,

$$\langle c_x^\dagger c_y\rangle \approx \frac{v_0}{L} Q_{x-y}^{(+)} + \frac{1}{L}\sum_{n=1}^{n^*} v_n \left(Q_{x-y+n}^{(+)} + Q_{x-y-n}^{(+)} \right) + \frac{i}{L} Q_{x-y}^{(-)} + \text{const.} \tag{5.28}$$

This approximation becomes exact in the limit of $n^* \to \infty$ taken after the thermodynamic limit.

In this way, the eigenstate expectation value of a local operator with a maximum range r is approximately written as a linear combination of $Q_n^{(\pm)}/L$ with $n \le r + n^*$, and this approximation becomes exact in the limit of $n^* \to \infty$. It implies that any local operator satisfies n_c-ETH in the limit of $n_c \to \infty$ after the thermodynamic limit. Thus, the strong generalized ETH has been proved.

[2] The value $\tilde{\varepsilon}(p) + \tilde{\varepsilon}(-p)$ is non-negative for all p. In the case in which $\tilde{\varepsilon}(p) + \tilde{\varepsilon}(-p)$ touches the p-axis, the functions (5.26) and (5.27) may not be L^1-integrable. In this case, the following arguments remain valid by replacing $\tilde{\varepsilon}(p) + \tilde{\varepsilon}(-p)$ by a constant $\delta_c > 0$ when $\tilde{\varepsilon}(p) + \tilde{\varepsilon}(-p)$ becomes smaller than δ_c, and taking the limit $\delta_c \to 0$ after $L \to \infty$ and $n_c \to \infty$.

5.4 Remarks

The strong generalized ETH proved in this work ensures that if the initial state is in a generalized shell constructed by local conserved quantities, the system relaxes to a steady state that is described by the GGE, either truncated or not. Since a physically relevant initial state, e.g., a state prepared by a quench, has subextensive fluctuations of macroscopic quantities, such an initial state is necessarily in a generalized shell. Therefore, a steady state after relaxation is described by a GGE in a translationally invariant noninteracting integrable system. Our results can be generalized to d-dimensional systems and noninteracting bosons.

In the previous studies, the validity of the GGE has been proved for noninteracting integrable models with translation invariance by requiring the cluster decomposition property for the initial state [100, 101]. In contrast, our result applies to dynamics with the initial state which can be any state in a single generalized shell. The cluster decomposition property does not hold for all of such states. Let us explain this point for the case of the usual thermalization and the energy shell. Consider an initially nonequilibrium state of a macroscopic uniform system, in which state the half of the system A is at a high temperature and the other half B is at a low temperature: $\rho_{\mathrm{high}}^{(A)} \otimes \rho_{\mathrm{low}}^{(B)}$. When there is interaction between the two subsystems A and B, the total system should eventually reach a state with a finite temperature T_c. We can consider another initially nonequilibrium state, in which this time the subsystem A is at low temperature and the subsystem B is at high temperature: $\rho_{\mathrm{low}}^{(A)} \otimes \rho_{\mathrm{high}}^{(B)}$. This state too should eventually reach the state with the finite temperature T_c. Now the mixed state $\rho_{\mathrm{mix}}^{(AB)} = \frac{1}{2}(\rho_{\mathrm{high}}^{(A)} \otimes \rho_{\mathrm{low}}^{(B)} + \rho_{\mathrm{low}}^{(A)} \otimes \rho_{\mathrm{high}}^{(B)})$ should also eventually reach a state at temperature T_c. However, $\rho_{\mathrm{mix}}^{(AB)}$ should violate the cluster decomposition property because it is a mixed state of macroscopically different states. Still, $\rho_{\mathrm{mix}}^{(AB)}$ should be in the energy shell around the energy corresponding to the temperature T_c. Therefore, the cluster decomposition property does not hold for all states in an energy shell. Similarly, the cluster decomposition property does not hold for all states in a single generalized shell. Therefore, our result shows that the GGE is valid for a wider class of initial states than expected previously.

It should be noted that the removal of the assumption of the cluster decomposition property is particularly important when we consider a spin model that is mapped to quadratic fermions, e.g., the transverse-field Ising chain and the XY chain. In these models, a physically realistic initial state should obey the cluster decomposition property *with respect to the spin operators*, but it is not obvious whether the same initial state obeys the cluster decomposition property *with respect to the fermion operators* [113].

We expect that our results can be generalized to interacting integrable systems by appropriately considering the quasilocal conserved quantities [111, 112] in such systems. We also hope that our proof of the generalized ETH may provide some insights for the challenge towards proving the usual ETH for nonintegrable systems.

Part II

Heating in integrable time-periodic systems

Chapter 6

Time-periodic systems

6.1 Importance of time-periodic systems

Closed quantum many-body systems driven by a time-periodic field have been studied actively in recent years [1, 30, 38–40]. The analysis of the steady states after a long time is one of the important questions in characterizing nontrivial quantum phenomena [45, 46, 48–53]. Periodically driven quantum systems gather attention both experimentally [76–80] and theoretically [31–35, 54–75] because of its potential of realizing novel physical phases, such as topological phases [49, 59–64, 68, 71, 72, 75–78, 81], by using simple time-dependent Hamiltonians. (See also Sec. 1.2.) This is called the Floquet engineering.

6.2 Floquet theory

There is a mathematical framework of the analysis of time-periodic systems, namely the Floquet theory [30]. When the Hamiltonian is periodic in time with the period T as $H(t+T) = H(t)$, the unitary time-evolution operator over a single period

$$U_{\mathrm{F}} = \mathcal{T} \exp\left(-i \int_0^T H(t)dt\right) =: e^{-iH_{\mathrm{F}}T} \tag{6.1}$$

defines an effective Hamiltonian H_{F}, which we call the Floquet Hamiltonian. Here, we denote the time-ordering operator by $\mathcal{T}$. At stroboscopic times $t = nT$ with n an integer, the time evolution is described by the static Hamiltonian H_{F}. Note that the Floquet Hamiltonian is dependent on the period: $H_{\mathrm{F}} = H_{\mathrm{F}}(T)$. We distinguish time-periodic systems as nonintegrable or integrable ones depending on whether H_{F} is nonintegrable or integrable, respectively. On the definition of integrability, see the review in Sec. 1.3.

6.3 Heating in time-periodic systems

In time-periodic systems, there is no conventional energy conservation because the Hamiltonian is time dependent [1] . Therefore, the energy of the system may rise, in other words, a heating may take place. It can be understood that the system absorbs energy from the external drive. In accordance with the Floquet engineering, the heating may break down the interesting quantum phases, and thus it is an important question whether the heating takes place and to what extent the system absorbs energy from the external driving [41–43]. Heating can be understood as the energy relaxation towards the maximum entropy state [37, 44–47] in the whole Hilbert space. From this perspective, it is also a fundamental issue of statistical physics, namely the thermalization [1–3].

We note that heating in closed systems is a phenomenon where a state approaches a high-temperature Gibbs state *in terms of expectation values of physical observables.* This point is in parallel with the recent discussion of thermalization in closed static systems; see also Sec. 1.1, Chap. 2, and Chap. 3.

Non-integrability is considered to play an essential role in heating of time-periodic systems. In this chapter, we review the prior understandings of the heating in nonintegrable time-periodic systems. On the other hand, the analysis on heating in integrable systems has been limited in preceding studies. We will review the prior discussions on heating in integrable time-periodic systems in Sec. 7.2.

6.3.1 Understanding of heating in nonintegrable time-periodic systems

Numerical studies [37,45,46,117–119] of relatively small nonintegrable systems have claimed that when the driving period T is small enough, a system does not heat up but stays at a finite temperature even after a long time, while when T is large enough the system heats up to (nearly) infinite temperature [2]. In the latter cases, the unlimited heating is believed to be related to the divergence of the high-frequency expansion [30,45] of the Floquet effective Hamiltonian, or the Floquet-Magnus (FM) expansion [120, 121]:

$$H_{\mathrm{F}}(T) = \sum_{n=0}^{\infty} T^n \Omega_n(T). \tag{6.2}$$

[1] Of course, the Floquet Hamiltonian H_{F} is a conserved quantity, but its effects on physical properties, i.e., properties that are obtained from the values of observables that can be measured in a usual setup, are generally nontrivial because H_{F} does not necessarily share properties with usual Hamiltonians obeying thermodynamics, as mentioned in Sec. 1.2.

[2] We note that in reality, a heating to the infinite temperature may be prevented by interactions with the surrounding environment.

The first few order terms are given by

$$\Omega_0(T) = \frac{1}{T}\int_0^T H(t_1)dt_1, \tag{6.3}$$

$$\Omega_1(T) = \frac{1}{2iT^2}\int_0^T dt_1 \int_0^{t_1} dt_2 [H(t_1), H(t_2)], \tag{6.4}$$

$$\Omega_2(T) = -\frac{1}{6T^2}\int_0^T dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 \Big([H(t_1), [H(t_2), H(t_3)]] + [H(t_3), [H(t_2), H(t_1)]]\Big), \tag{6.5}$$

and the general form is given by [122–124]

$$\begin{aligned}\Omega_n =& \frac{1}{(n+1)^2}\sum_\sigma (-1)^{n-\Theta(\sigma)} \frac{\Theta(\sigma)!(n-\Theta(\sigma))!}{n!} \times \frac{1}{i^n T^{n+1}} \\ &\times \int_0^T dt_{n+1} \dots \int_0^{t_3} dt_2 \int_0^{t_2} dt_1 \left[H(t_{\sigma(n+1)}), \left[H(t_{\sigma(n)}), \dots, \left[H(t_{\sigma(2)}), H(t_{\sigma(1)})\right] \dots\right]\right],\end{aligned} \tag{6.6}$$

where σ denotes the permutation of indices and $\Theta(\sigma) := \sum_{i=1}^n \theta(\sigma(i+1) - \sigma(i))$, where $\theta(\cdot)$ is the step function.

The nth-order term $\Omega_n(T)$ includes nested commutators of the time-dependent Hamiltonian with order n. In particular, the first term is equal to the time average over one period of the time-dependent Hamiltonian, which we refer to as H_{ave}:

$$\Omega_0(T) = H_{\mathrm{ave}} := \frac{1}{T}\int_0^T H(t)dt. \tag{6.7}$$

Throughout this thesis, we refer to the expectation value of the operator H_{ave} as the energy of the periodically driven system; this is a convention often adopted in the studies of time-periodic systems. If the period T is sufficiently small, the Floquet Hamiltonian may be approximated by the average Hamiltonian $H_{\mathrm{F}} \approx H_{\mathrm{ave}}$, and therefore the system should remain in a low-energy state if we start from the ground state of H_{ave}. However, the convergence of the FM expansion (6.2) is generally not assured for large periods. A general sufficient condition for the convergence is given by

$$\int_0^T ||H(t)||dt \le \xi, \tag{6.8}$$

where ξ is a universal constant [121, 125–128]. It implies that the convergence is ensured only for $T \lesssim 1/\|H(t)\|$ with $\|\cdots\|$ the operator norm.

When the FM expansion diverges, the Floquet Hamiltonian is no longer close to H_{ave} and higher-order terms become dominant. In the periodically driven nonintegrable systems, the spectral structure is known to resemble that of a random matrix [45, 47]. This implies that the steady state is given by a random state in the total Hilbert space, namely the infinite-temperature state [21]. This leads to the belief that the two regimes of different extents of heating seen in the numerical studies of finite nonintegrable systems, explained above, may be bordered by the divergence point of the FM expansion.

Since the norm $||H(T)||$ for nonintegrable systems diverges in the thermodynamic limit, the maximum driving period in the region where the convergence of the FM expansion is ensured by Eq. (6.8) converges to zero in the thermodynamic limit. Although there is no general analytical method of obtaining an actual divergence point, it is believed that generally there exists an actual divergence point which indeed converges to zero in the thermodynamic limit. The divergence of the expansion is observed in numerical calculations [124, 129]. From these arguments, it is expected that macroscopic nonintegrable systems heat up to infinite temperature at any nonzero driving periods in the long-time limit, although the time-scale may be extremely long [124, 129–133].

We note that according to the adiabatic theorem, the heating rate within the unit time should get smaller as the driving period gets larger. Nevertheless, this is compatible with the seemingly opposite conclusion of heating to infinite temperature, because now the infinite-time limit is taken. We also note that in numerical calculations, the infinite-time limit of the expectation value of an observable can be calculated by dropping the off-diagonal elements of the observable in the eigenbasis of the Floquet Hamiltonian.

Chapter 7

Integrable time-periodic systems

7.1 Classes of integrable time-periodic systems

As explained in sec. 1.3.1, integrable time-periodic systems are defined as time periodic systems whose effective Hamiltonian H_F is integrable; see sec. 1.3 for the definition of integrability. The simplest case of such systems is where the time-dependent Hamiltonian $H(t)$ is quadratic at each time t. The Hamiltonian in the case is written as

$$H(t) = \sum_{i,j=1}^{L} \left(a_i^\dagger \mathcal{M}_{ij}(t) a_j + a_i^\dagger \mathcal{N}_{ij}(t) a_j^\dagger + \text{H.c.} \right), \tag{7.1}$$

where $a^\dagger$ and a are the creation and annihilation operators, respectively, that satisfy either the fermionic or bosonic commutation relations. In this case, the Floquet Hamiltonian H_{F} is also quadratic and can be mapped to the free-fermion or free-boson systems. Thus it is obviously of a class of integrable time-periodic systems. Recently, several other classes of integrable time-periodic systems are presented [134], including those that are related to interacting integrable quantum spin chains.

7.2 Prior discussions for heating in integrable time-periodic systems

In integrable time-periodic systems, there are apparent conserved quantities as many as the degree of freedom of the system. The quantum dynamics is restricted in the state space characterized by them. This has led to an expectation on heating in integrable time-periodic systems: the unlimited heating as is discussed for nonintegrable time-periodic systems does not take place, and the system converges to a nontrivial steady state [53,134–138]. Indeed, there has been no report on heating to infinite temperature for integrable time-periodic systems, without additional conditions such as a random noise [139]. Nonetheless, the connection between the heating and the integrability has been only intuitive; It was not known whether heating to the infinite temperature may take place, and if so, whether there exists some transition or a crossover.

Another point that has been subtle in integrable time-periodic systems was the relation between the property of the steady state and the divergence of the Floquet-Magnus expansion. The Floquet-Magnus expansion may diverge not only in nonintegrable time-periodic systems but in integrable time-periodic systems too, although the nature of the convergence radius is distinctly different from that of the nonintegrable time-peiodic systems, as will be explained in the next section. It is a natural question to ask whether the divergence of the Floquet-Magnus expansion affects in any way the property of the steady state, especially the extent of heating, like in nonintegrable time-periodic systems.

The above questions are summarized in a recent review [135] of time-periodic systems. These questions are exactly what we give an answer to in Chap. 8.

7.3 Generalized Gibbs ensemble for integrable time-periodic systems

It has been proposed for integrable time-periodic systems that its steady state is given by a form of the generalized Gibbs ensemble [53], which was originally discussed in the static systems, as is explained in Sec. 1.3.1. It is occasionally referred to as "periodic Gibbs ensemble" or the "Floquet GGE." The validity of the GGE for time-periodic systems is not so well established as that of the GGE in static systems. This is because the general property of the Hamiltonian that determines the dynamics is distinctly different in general between static and time-periodic systems, as mentioned in Sec. 1.3.1. Nonetheless, a relatively elaborate analysis has been done in the case where the time dependent Hamiltonian $H(t)$ is quadratic [53].

We here explain the analysis of quadratic fermionic time-periodic system of the case in which the total particle number is conserved. The system of the numerical study we present in Chapter. 8 is included in this case. We consider the following Hamiltonian:

$$H(t) = \sum_{i,j=1}^{L} \left(a_i^\dagger \mathcal{M}_{ij}(t) a_j + \text{H.c.} \right), \tag{7.2}$$

where $a^\dagger$ and a are the creation and annihilation operators, respectively, which satisfy the fermionic commutation relations and L denotes the system size. In this case, the Floquet Hamiltonian H_{F} is also quadratic and can be mapped to free-fermion systems (see Appendix A). This systems has L pieces of apparent conserved quantities denoted as

$$\hat{\mathcal{I}}_p = f_p^\dagger f_p \tag{7.3}$$

for $p = 1, 2, \ldots, L$, where $f_p^\dagger$ and f_p are eigenmodes of H_F, namely $H_\mathrm{F} = \sum_{p=1}^L \epsilon_p f_p^\dagger f_p$ with $\{\epsilon_p\}_{p=1}^L$ the quasi-energies of H_F. The dynamics is constrained in the Hilbert space which conserves all of $\{\hat{\mathcal{I}}_p\}_{p=1}^L$. We have $\sum_{p=1}^L f_p^\dagger f_p |\psi(t)\rangle = N|\psi(t)\rangle$ for all t, where N is the number of modes occupied in the initial state, which we refer to as the particle number. We define the infinite-temperature state as the uniform mixing of all the states with a fixed particle number N. That is, the infinite-temperature state, which we denote by $\mathbf{1}_{(N,L)}$, is proportional to the projection operator $P_{N,L}$ to the Hilbert space with the particle number N.

Let us here explain the divergence of the Floquet-Magnus expansion (see Sec. 6.3.1) for the present integrable time-periodic systems. The convergence of the FM expansion is ensured for a wider region of T in the integrable cases than in nonintegrable systems. In the present integrable time-periodic systems, the convegence of the FM expansion is ensured for $T \lesssim 1/\|\mathsf{M}(t)\|$, where $\mathsf{M}(t)$ is the $L \times L$ matrix which expresses the single-particle Hamiltonian with its norm $\|\mathsf{M}(t)\|$ remaining finite even in the thermodynamic limit; see Appendix A. In the integrable cases, the Floquet Hamiltonian H_F always commutes with the conserved quantities and is far from the random matrix in the total Hilbert space.

It has been proposed [53] that the steady state of the system given by Eq. (7.2) is given by a GGE of the form

$$\rho_\mathrm{GGE} = \mathcal{Z}^{-1} \exp\left(-\sum_{p=1}^{L} \Lambda_p \hat{\mathcal{I}}_p \right), \tag{7.4}$$

with $\mathcal{Z}$ the normalization constant. We refer to the coefficients $\{\Lambda_p\}_{p=1}^L$ as "the effective temperatures" for the conserved quantities $\{\hat{\mathcal{I}}_p\}_{p=1}^L$. The effective temperature Λ_p is calculated by equating the expectation values of the conserved quantity $\hat{\mathcal{I}}_p = f_p^\dagger f_p$ for the initial pure state and the GGE given by Eq. (7.4) as in

$$\langle \psi_0 | f_p^\dagger f_p | \psi_0 \rangle = \frac{1}{e^{\Lambda_p} + 1}, \quad p = 1, 2, \ldots, L, \tag{7.5}$$

where $\langle \psi(t) | f_p^\dagger f_p | \psi(t) \rangle = \langle \psi_0 | f_p^\dagger f_p | \psi_0 \rangle$ holds, with $|\psi_0\rangle$ and $|\psi(t)\rangle$ denoting the initial state and the state at time t, respectively. Thus, for a fixed initial state $|\psi_0\rangle$, $\{\Lambda_p\}_{p=1}^L$ is dependent on $\{\hat{\mathcal{I}}_p\}_{p=1}^L$, which varies for different Floquet Hamiltonians H_F.

We stress that the steady state of the present system is expected to be given by the GGE as in Eq. (7.4) for all driving periods regardless of the convergence of the FM expansion (although $\{\Lambda_p\}_{p=1}^L$ depend on the driving period T because $\hat{\mathcal{I}}_p = f_p^\dagger f_p$ on the left-hand side of (7.5) is an eigenmode of the Floquet Hamiltonian, which depends on T). Still, the quantum expectation values of physical quantities including the energy H_ave after a long time may look like those at the infinite temperature when the FM expansion diverges. This is what we mainly examine in Chap. 8.

Chapter 8

Numerical study of heating in concrete integrable time-periodic systems

In this chapter, we present our results of the numerical study of the steady state of several specific integrable time-periodic models. After beginning with the introduction of the models, we calculate the rise in energy of the steady state compared to the initial state taken as the lowest energy state. We then conduct a scaling analysis of the rise in energy, with respect to the system size L and driving period T. As an approach to the steady state from a different point of view, we also calculate the effective temperatures of the GGE. We finally present a discussion and a conclusion.

8.1 Model and setup

We consider a spin-1/2 chain with L sites under the open boundary conditions. (We presume that the boundary condition is not critical to the conclusion of our calculation, because we focus on the bulk properties.) We periodically switch the system Hamiltonian back and forth between two Hamiltonians H_1 and H_2. The time evolution operator over one period is

$$U_{\mathrm{F}}(T) = e^{-iH_2T/2}e^{-iH_1T/2}. \tag{8.1}$$

Here, we choose H_1 as the XX model Hamiltonian and H_2 as the Hamiltonian of the external field along z-axis:

$$H_1 = \sum_{i=1}^{L-1} \left(\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y \right), \tag{8.2}$$

$$H_2 = \sum_{i=1}^{L} h_i \sigma_i^z, \tag{8.3}$$

where we consider three types of $\{h_i\}_{i=1}^L$: a quasi-periodic field $h_i = \sin\left(2\sqrt{2}\pi \cdot i\right)$, a random field with $\{h_i\}_{p=1}^L$ given by a random Gaussian with the unit standard deviation, and the staggered field $h_i = (-1)^i$. The average Hamiltonian in Eq. (6.7) is now given by

$$H_{\mathrm{ave}} = (H_1 + H_2)/2. \tag{8.4}$$

After the Jordan-Wigner transformation, both the two Hamiltonians H_1 and H_2 can be written in quadratic forms of fermionic operators as

$$\sum_{i,j=1}^{L} a_i^\dagger \mathcal{M}_{ij} a_j. \tag{8.5}$$

Therefore, the unitary operator (8.1) defines an integrable Floquet Hamiltonian; see Appendix A.

In order to observe the heating behavior clearly, we choose the ground state of H_{ave} as the initial state $|\psi_0\rangle$. We have numerically confirmed that the particle number N of the initial state is about $L/2$ in the present models. We denote the infinite-time average of operators by $\overline{\langle \cdots \rangle}$. In the following, we consider the infinite-time average of the energy density $\overline{\langle H_{\mathrm{ave}} \rangle}/L$ and the effective temperatures $\{\Lambda_p\}_{p=1}^L$ for conserved quantities $\{\hat{\mathcal{I}}_p\}_{p=1}^L$ in (7.3).

8.2 Energy of the steady state

First we calculate the expectation value of the energy density H_{ave}/L for the steady state after infinite time. The energy at time $t = mT$, $m \in \mathbb{N}$ (i.e., time after m periods) is

$$\langle H_{\mathrm{ave}} \rangle = \langle \psi_0 | (U_{\mathrm{F}}^\dagger)^m H_{\mathrm{ave}} (U_{\mathrm{F}})^m | \psi_0 \rangle. \tag{8.6}$$

Note that U_{F} is dependent on the driving period as $U_{\mathrm{F}}(T) = e^{-iH_{\mathrm{F}}(T)T}$; see Sec. 6.2. The infinite-time average of the energy density $\overline{\langle H_{\mathrm{ave}} \rangle}/L$ is given by dropping the off-diagonal terms of H_{ave} represented in the basis of the eigenstates of H_{F} [91]. We compare $\overline{\langle H_{\mathrm{ave}} \rangle}/L$ with the expectation value in the infinite-temperature state $\mathbf{1}_{(N,L)}$.

We note that we consider heating to the infinite temperature as a phenomenon where the steady state is equivalent to $\mathbf{1}_{(N,L)}$ *in terms of expectation values of physical observables* (see also Sec. 6.3). We analyze H_{ave} as a specific physical observable, but also expect similar behaviors for other local observables too.

We show in Fig. 8.1 the energy density difference

$$\Delta u(T) := \overline{\langle H_{\text{ave}} \rangle}/L - \text{Tr}[\mathbf{1}_{(N,L)} H_{\text{ave}}]/L \tag{8.7}$$

against the driving period T for the system sizes $L = 30, 60, 100$. The vertical line indicates the period where we numerically detected the divergence of the FM expansion for $H_{\text{F}}(T)$; see Appendix B.1 Fig. B.1 for details. In each panel of Fig. 8.1, we can see a sharp rise of $\Delta u(T)$ around $T \approx 1$, which is close to the divergence point. However, the size dependence suggests that the energy absorption remains finite above the divergence point $T \gtrsim 1$ in the thermodynamic limit $L \to \infty$.

As the driving period increases, a qualitative difference appears between Figs. 8.1(a,b) and Fig. 8.1(c). In the cases of the quasi-periodic and random fields, Figs. 8.1(a) and (b) indicate that the deviation $|\Delta u|$ decays as T and L increase. On the other hand, in the case of the staggered field (Fig. 8.1(c)), we clearly see that the infinite-time average of the energy deviates from the infinite-temperature value for all data points.

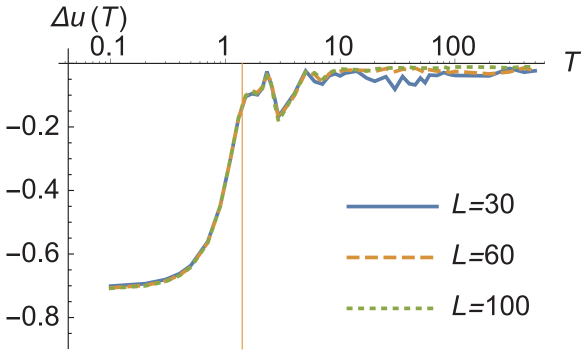
8.3 Scaling analysis

For the former cases, we calculated $\Delta u(T)$ for larger sizes than in Figs. 8.1 (a,b). We found good scaling as in Fig. 8.2 (see also Appendix B.2 Fig. B.2, which shows the data plotted with pre-scaled axes. We obtained Fig. 8.2 by collapsing the data in the region $T \geq 20$ of Fig. B.2. The scaling breaks in the region with smaller values of T.); the data points lie on a single curve for all L for the shown region of periods when we plot $|\Delta u| \times L$ against $T/\sqrt{L}$. (We take the absolute value $|\Delta u|$ instead of Δu to plot in the logarithmic scale.)

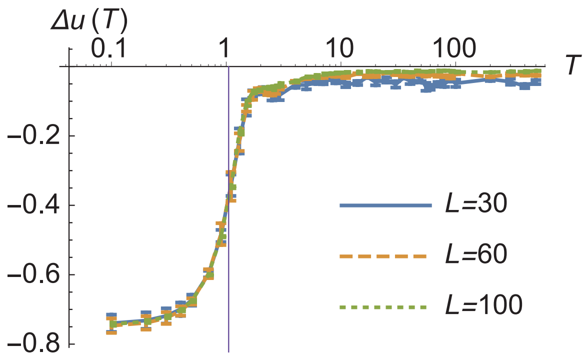
This scaling plot means that the quantity $Q := |\Delta u|$ is given by a scaling function $\tilde{Q}$ in the form

$$Q(T, L) = L^{-1}\tilde{Q}(TL^{-1/2}). \tag{8.8}$$

The curve implies that for a finite system the heating saturates before reaching the infinite-temperature value even in the limit $T \to \infty$; the part of the curve which is nearly parallel to the horizontal axis corresponds to the region where the saturation takes place. By the standard dynamical scaling analysis (see for example Ch.2 of Ref. [140]), we conclude that the finite-size data should converge to the infinite-size limit $Q = 0$ for $T = \infty$ as $Q \propto 1/L$. For finite but large T, we have $Q(T, L) = T^{-2}[(TL^{-1/2})^2\tilde{Q}(TL^{-1/2})]$, and hence conclude that $Q \propto T^{-2}$ holds in the infinite-size limit $L \to \infty$. (The exponent -2 corresponds to the gradient of the part of the curve which is not parallel to the horizontal axis. See also



(a)



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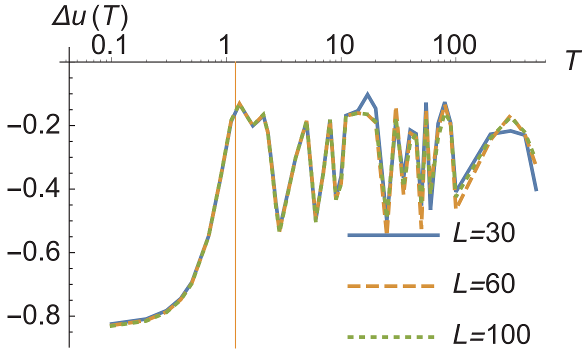


(c)

Figure 8.1: Deviation of the energy density from the value at the infinite temperature. We set $\{h_i\}$ in Eq. (8.3) as (a) the quasi-periodic field, (b) the random Gaussian field with four random samples, and (c) the staggered field; see the description below Eq. (8.3). Each line (and color) shows the result for the corresponding system size. The amount of the energy absorption drastically changes near $T \approx 1$. The vertical line indicates the period where we detected the divergence of the FM expansion.

Appendix B.2 Fig. B.2.) Therefore the system heats up to infinite temperature in the limit $L \to \infty$ and $T \to \infty$.

8.4 Effective temperatures in the GGE

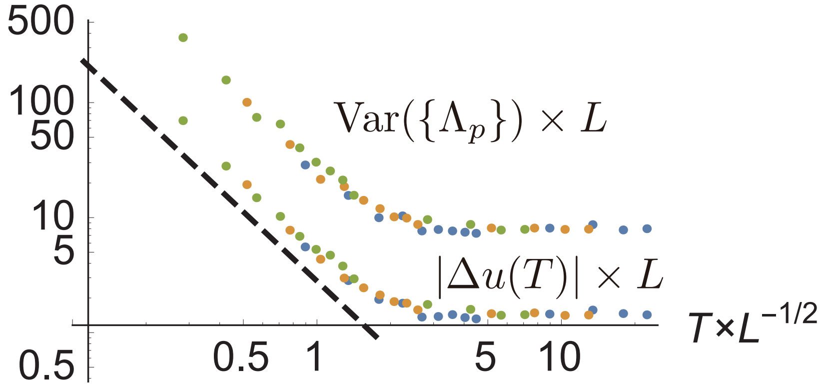
Next we examine different quantities to confirm that the steady state resembles the infinite-temperature state for observables other than the energy. For the purpose, we consider the effective temperatures for the L pieces of conserved quantities $\hat{\mathcal{I}}_p = f_p^\dagger f_p$, namely Λ_p for $p = 1, \ldots, L$ given in Eq. (7.4). For the infinite-temperature state $\mathbf{1}_{(N,L)}$, all the expectations $\mathrm{Tr}(\mathbf{1}_{(N,L)}\hat{\mathcal{I}}_p)$ for $p = 1, 2, \ldots, L$ have the same value. Hence, if all of $\{\Lambda_p\}_{p=1}^L$ in the GGE have the same value, the state (7.4) reduces to the infinite-temperature state for a fixed particle number N. We therefore analyze the variance among $\{\Lambda_p\}_{p=1}^L$ from the expectation, which we denote as $\mathrm{Var}(\{\Lambda_p\}) := \frac{1}{L}\sum_{p=1}^L(\Lambda_p - \overline{\Lambda})^2$ with $\overline{\Lambda} := \frac{1}{L}\sum_{p=1}^L \Lambda_p$. The decrease of $\mathrm{Var}(\{\Lambda_p\})$ means the approach of the steady state to the infinite temperature.

After fixing L and T, we can obtain the values of $\{\Lambda_p\}_{p=1}^L$ by numerically computing the left-hand side of Eq. (7.5). The value $\langle\psi_0|f_p^\dagger f_p|\psi_0\rangle$ can be computed by expanding $f_p^\dagger$ and f_p in terms of the eigenmodes of H_{ave}.

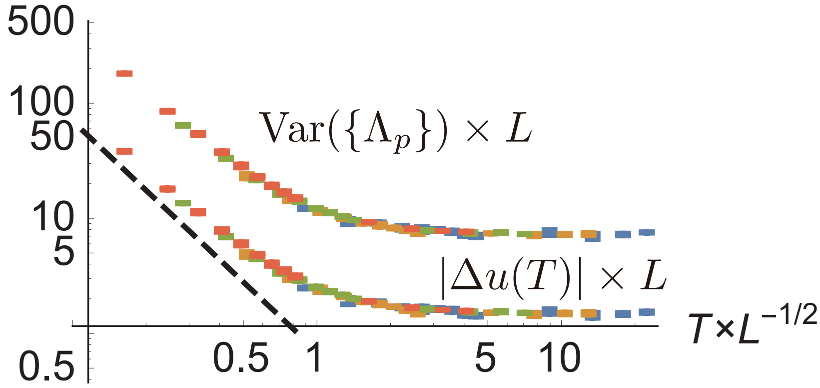
We conduct the scaling analysis again in order to analyze how $\mathrm{Var}(\{\Lambda_p\})$ approaches zero as L and T increase. As in Fig. 8.2, we find that $\mathrm{Var}(\{\Lambda_p\})$ follows the same scaling as $|\Delta u|$. (In the Appendix B.2 Fig. B.3, we show the T-dependence of $\mathrm{Var}(\{\Lambda_p\})$ for various system sizes L.) This reveals that the GGE in Eq. (7.4) converges to the infinite-temperature state in the limits of $L \to \infty$ and $T \to \infty$. This gives another piece of evidence for the heating to the infinite-temperature state.

8.5 Discussion

Here we discuss why a qualitative difference appeared between the cases in which $\{h_i\}$ in H_2 was (a) quasi-periodic or (b) random fields, and (c) a staggered field. The extent of heating may be explained by the degree of mixing in the one-body state space under the basis of the wave number. The first Hamiltonian H_1, namely the XX model, conserves the wave number of the state. In order to bring the initial state close to the infinite temperature, it requires for the second Hamiltonian H_2 to mix various wave numbers into the state $|\psi(t)\rangle$. In the cases (a) and (b), H_2 causes mixing of modes with many different wave numbers, while in the case of (c), H_2 only moves the occupation of a mode to another mode with a wave number difference π. We infer that this is the reason why in the case of (c), no extensive heating took place as anticipated conventionally, while in the cases of (a) and (b), extensive heating, especially heating to the infinite temperature in the asymptotic sense, took place in spite of the system being integrable. We expect that extensive heating



(a)



(b)

Figure 8.2: Scaling plots of $|\Delta u(T)|$ and $\mathrm{Var}(\{\Lambda_p\})$. We set $\{h_i\}$ in Eq. (8.3) as (a) the quasi-periodic fields and (b) the random Gaussian field with four random samples. The driving periods are $T = 20,\ 30,\ 40,\ 50,\ 60,\ 70,\ 80,\ 90,\ 100,\ 200,\ 300,\ 400,\ 500$. The system sizes are $L = 500,\ 1500,\ 5000$ for the quasi-periodic field and $L = 500,\ 1500,\ 5000,\ 15000$ for the random field. (Different colors indicate different system sizes.) The broken line indicates the behavior T^{-2}.

takes place for other driving fields too if the field mixes various enough wave numbers into the state $|\psi(t)\rangle$.

Let us comment on the driving-period dependence of the extent of heating in the cases (a) and (b). When the driving period T is small enough, H_{ave} approximates the Floquet Hamiltonian, and thus its degree of mixing of modes with different wave numbers is small, resulting in a small amount of heating. On the other hand, for the large driving periods where the FM expansion diverges, it should be a challenging problem to evaluate the extent of heating analytically since the Floquet Hamiltonian is determined through the nontrivial contributions of H_1 and H_2. We note that it is a nontrivial behavior that the heating to the infinite temperature does not take place for finite driving periods, even when the driving period is larger than the divergence point of the Floquet Magnus expansion. We also stress that it is a novel finding in time-periodic systems that any scaling behavior in quantum states far from equilibrium exists, having the driving period T as one of its scaling variables.

Let us here mention the relevance to experiments of the present models. The time-periodic modulation of fermions with nearest-neighbor hopping and quasi-random potential has been achieved in an experiment [80]. An alternative way of realizing the present system is to use hard-core bosons, whose Hamiltonian can be mapped to the Hamiltonian of free fermions [53]. Hard-core bosons are also achieved in an experiment of ultracold atoms in optical lattices [141]. We thus expect that the scaling of heating expressed by Eq. (8.8) should be verified experimentally in these systems.

Chapter 9

Conclusions

In this thesis, we considered the long-time steady state of closed integrable systems. In Part I, we considered static integrable systems. We questioned the foundation of the statistical ensemble called the generalized Gibbs ensemble (GGE), which was recently proposed as a description of the steady state of integrable systems. In Part II, on the other hand, we considered time-periodic integrable systems. We explored the heating property in the long-time limit of specific integrable systems. While a form of GGE, namely the Floquet GGE, has been proposed in preceding studies as a description of the long-time steady state of time-periodic systems, we did not go into the foundation of the Floquet GGE in this thesis. In the following, we summarize and make concluding remarks for each Parts, followed by future perspectives.

In Chapters 2 and 3, we reviewed the analysis of thermalization developed in recent years. In Chapter 2, we showed that by considering the expectation values of observables in the long-time limit, a system can be understood to equilibrate under unitary evolution, under the conditions of nondegenerate energy gaps and the large effective dimension. In Chapter 3, we reviewed the recently proposed eigenstate thermalization hypothesis (ETH). The ETH states that all the individual eigenstates in the energy shell represent a thermal state. While ETH is still a hypothesis in generic systems, its validity ensures that the equilibrium state is in fact the thermal state described by the Gibbs ensemble. The validity of ETH is confirmed by many numerical calculations. We stressed that a deformed version of the ETH, namely the weak ETH, which states that *almost all* of the eigenstates in the energy shell represents a thermal state, does not ensure thermalization. Only the original ETH, occasionally called the strong ETH, ensures thermalization.

In Chapter 4, we reviewed the understanding on the equilibrium state of integrable systems. In contrast to nonintegrable systems, it is known that integrable systems do not thermalize. It was proposed recently that its steady state is given by the GGE instead. The GGE is constructed in terms of the conserved quantities of the system. It has been expected that more local conserved quantities are more important in the description of the steady state. In preceding studies, the validity of GGE was numerically confirmed, as well as proved for translationally invariant noninteracting systems under the assumption of the clustering property with respect to the relevant fermion/boson operators of the initial state.

In Chapter 5, we questioned the foundation of GGE. We defined a Hilbert subspace which we call the generalized shell, using the local conserved quantities of the system. The generalized shell can be understood as a generalization of the energy shell. Based on the generalized shell, we formulated a generalized version of the ETH in the strong sense. The generalized ETH ensures equilibration to the GGE, which is in parallel to the fact that the usual (strong) ETH ensures equilibration to the Gibbs state. We analytically proved the validity of the generalized ETH for translationally invariant noninteracting systems.

Our proof ensures equilibration to the GGE for arbitrary initial states that have subextensive fluctuations of local conserved quantities. Such initial states are of a wider class than initial states satisfying the clustering property, for which the validity of GGE was proved in preceding studies. This is especially important in spin systems that can be mapped to noninteracting systems, because while a physically realistic initial state should obey the cluster-decomposition property with respect to the spin operators, it is not obvious whether the same initial state obeys the cluster-decomposition property with respect to the fermion operators.

We expect that our generalized ETH is a general mechanism for the validity of GGE in integrable systems, and can be generalized for interacting integrable systems by appropriately considering the quasilocal conserved quantities, which have been acknowledged to play an important role in the steady state of interacting integrable systems. We hope that our proof of the generalized ETH may provide some insights for the challenge towards the proof of the usual ETH in generic systems.

We proceed to the summary and concluding remarks for Part II. In Chapter 6, we reviewed generic time-periodic systems. In the Floquet theory, time-periodic systems can be mapped to a problem of a static effective Hamiltonian. The study of long-time steady states of time-periodic systems is a problem of equilibration under the effective Hamiltonian. It is also important in applications, because time-periodic systems may realize novel physical phases by inducing simple time-periodic modulation on materials. Understanding the heating behavior is particularly important, because the heating may break the interesting physical phases. In nonintegrable time-periodic systems, it is expected that heating to the infinite temperature is universal in the long-time limit. In Chapter 7, we reviewed prior understanding of integrable time-periodic systems. Integrable time-periodic systems are defined as time-periodic systems whose effective Hamiltonian is integrable. A form of GGE, called the Floquet GGE is proposed as a description of its long-time steady state, although its foundation is still not firm. Integrable time-periodic systems are expected to be realizable with current techniques on cold atoms and modulation of optical lattices. In prior discussions, heating to the high temperature was not expected in integrable time-periodic systems because the conserved quantities restrict the dynamics in the Hilbert space. However, this was only an intuitive discussion.

In Chapter 8, we numerically studied the heating behavior in specific integrable systems. We clarified that heating to the high temperature can actually take place in integrable time-periodic systems too. We found for several models that the amount of heating rises drastically near a threshold where the Floquet-Magnus expansion diverges. We found for the amount of heating in the low-frequency regime a scaling behavior as to the driving period and the system size. We revealed that the system heats up to the infinite temperature in the limit of infinite system size and driving period. We also found that the Floquet GGE approached the infinite-temperature state as the amount of heating rose. We also showed the results of a case where a model that does not heat up close to the infinite temperature in all regimes. We discussed the origin of the distinct difference in the heating behaviors of the two cases and attributed it to the extent of mixing in the state space in the basis of wave numbers.

Finally, we present future perspectives. There are still many problems to be resolved towards the full understanding of equilibration and thermalization. As we mentioned earlier, the generalization to interacting integrable systems of the generalized ETH that we formulated is an important task. It is also a future problem to clarify whether the assumption of the translation invariance and the locality of the Hamiltonian that we assumed in our proof are necessary. Considering the case of nonlocal Hamiltonian is important in validating the relaxation to the Floquet GGEin the low-frequency regime of time-periodic systems, where the effective Hamiltonian generally becomes nonlocal. In generic systems not restricted to integrable systems, the proof of usual ETH remains an open problem. The time scale of equilibration, as well as the prethermalization, are also important subjects.

As for the time-periodic systems, analytic derivation of the nontrivial scaling exponents in $Q \propto L^{-1}$ and $Q \propto T^{-2}$ remains an open question. Our results indicate that the Floquet Hamiltonian H_{F} resembles a kind of random matrix in the limit of $T \to \infty$ and $L \to \infty$ for the quasi-periodic and random fields. The present scalings may be explained by analyzing the difference between the random matrix and the time evolution operator over one period $U_{\mathrm{F}}(T)$ for finite T and L if we can find an appropriate quantitative index. Analysis for other classes of time-periodic systems may be an interesting problem. We expect that the scalings that we found may form a universality class and appear in other integrable time-periodic systems. We also note that a similar scaling analysis may be helpful also for nonintegrable time-periodic systems for further studying its finite-size behavior. Clarifying the time scale of heating remains to be solved. As mentioned above, the validity and the conditions of the Floquet GGE still remain as open problems. Exploring equilibration and the steady states of other setups out of the class of closed static systems, besides time-periodic systems, constitutes a large set of issues to be challenged. A paradigmatic class of such is open systems, including those with a constant current.

Appendix A

One-period unitary operator of time-periodic free fermion systems

Here we show that the calculation of the one-period unitary operator U_{F} of a free-fermion system can be reduced to solving the Floquet problem of an $L \times L$ operator. This calculation is necessary for finding the eigenmodes of the Floquet Hamiltonian.

Consider the time-dependent Hamiltonian

$$H(t) = \sum_{n,m=1}^{L} M_{nm}(t) a_n^\dagger a_m, \tag{A.1}$$

where a_m is the annihilation operator of a fermion. Denoting the column vector of the annihilation operator as $\boldsymbol{a}$, we can express this Hamiltonian as

$$H(t) = \boldsymbol{a}^\dagger \mathsf{M}(t) \boldsymbol{a}, \tag{A.2}$$

where $\mathsf{M}(t)$ denotes a matrix whose elements are given by $(\mathsf{M}(t))_{nm} = M_{nm}(t)$.

The one-period unitary operator U_{F} is defined by

$$U_{\mathrm{F}} = \mathcal{T} e^{-i \int_0^T H(t) dt} = e^{-i H_{\mathrm{F}} T}, \tag{A.3}$$

where $\mathcal{T}$ denotes the time-ordering operator. The Floquet Hamiltonian is also quadratic as in

$$H_{\mathrm{F}} = \boldsymbol{a}^\dagger \mathsf{M}_{\mathrm{F}} \boldsymbol{a}. \tag{A.4}$$

In the following, we show how to obtain M_{F}.

We define

$$\boldsymbol{a}^\dagger(t) \equiv U_t \boldsymbol{a}^\dagger U_t^\dagger, \tag{A.5}$$

where $U_t = \mathcal{T} e^{-i \int_0^t H(s) ds}$. Defining $\mathsf{A}(t)$ as $\boldsymbol{a}^\dagger(t) =: \boldsymbol{a}^\dagger \mathsf{A}(t)$, we have

$$\boldsymbol{a}^\dagger \frac{d\mathsf{A}(t)}{dt} = \frac{d}{dt}(U_t \boldsymbol{a}^\dagger U_t^\dagger) = -i[H(t), \boldsymbol{a}^\dagger \mathsf{A}(t)] = -i \boldsymbol{a}^\dagger \mathsf{M}(t) \mathsf{A}(t) \tag{A.6}$$

with the usage of the equality $[H(t), \boldsymbol{a}^\dagger] = \boldsymbol{a}^\dagger \mathsf{M}(t)$. Therefore, we obtain

$$\frac{d\mathsf{A}(t)}{dt} = -i\mathsf{M}(t)\mathsf{A}(t). \tag{A.7}$$

The solution of Eq. (A.7) under the condition $A(0) = 1$ is

$$\mathsf{A}(t) = \mathcal{T} e^{-i\int_0^t \mathsf{M}(s)ds}. \tag{A.8}$$

Therefore,

$$\boldsymbol{a}^\dagger(t) = U_t \boldsymbol{a}^\dagger U_t^\dagger = \boldsymbol{a}^\dagger \mathcal{T} e^{-i\int_0^t \mathsf{M}(s)ds} \tag{A.9}$$

holds.

Now we show how M_F can be calculated from $\mathsf{M}(t)$. The basis state of an N-particle state is given by

$$a_{i_1}^\dagger a_{i_2}^\dagger \dots a_{i_N}^\dagger |0\rangle, \tag{A.10}$$

where $\{i_1, i_2, \dots i_N\}$ is a set of integers which satisfies $1 \le i_1 < i_2 < \dots < i_N \le L$, and $|0\rangle$ is the vacuum. We can determine M_F by observing how the above state is transformed by U_F. It is expressed as

$$U_\mathrm{F} a_{i_1}^\dagger a_{i_2}^\dagger \dots a_{i_N}^\dagger |0\rangle = U_\mathrm{F} a_{i_1}^\dagger U_\mathrm{F}^\dagger \cdot U_\mathrm{F} a_{i_2}^\dagger U_\mathrm{F}^\dagger \dots U_\mathrm{F} a_{i_N}^\dagger U_\mathrm{F}^\dagger \cdot U_\mathrm{F}|0\rangle. \tag{A.11}$$

From $U_\mathrm{F}|0\rangle = |0\rangle$ and $U_\mathrm{F}\boldsymbol{a}^\dagger U_\mathrm{F}^\dagger = \boldsymbol{a}^\dagger(T) = \boldsymbol{a}^\dagger \mathcal{T} e^{-i\int_0^T \mathsf{M}(s)ds}$, we obtain

$$U_\mathrm{F} a_{i_1}^\dagger a_{i_2}^\dagger \dots a_{i_N}^\dagger |0\rangle = (\boldsymbol{a}^\dagger \mathcal{T} e^{-i\int_0^T \mathsf{M}(s)ds})_{i_1} \cdot (\boldsymbol{a}^\dagger \mathcal{T} e^{-i\int_0^T \mathsf{M}(s)ds})_{i_2} \cdots (\boldsymbol{a}^\dagger \mathcal{T} e^{-i\int_0^T \mathsf{M}(s)ds})_{i_N} |0\rangle. \tag{A.12}$$

On the other hand, putting $U_\mathrm{F} = e^{-i\boldsymbol{a}^\dagger \mathsf{M}_\mathrm{F} \boldsymbol{a} T}$, we obtain

$$e^{-i\boldsymbol{a}^\dagger \mathsf{M}_\mathrm{F} \boldsymbol{a} T} a_{i_1}^\dagger a_{i_2}^\dagger \dots a_{i_N}^\dagger |0\rangle = (\boldsymbol{a}^\dagger e^{-i\mathsf{M}_\mathrm{F} T})_{i_1} \cdot (\boldsymbol{a}^\dagger e^{-i\mathsf{M}_\mathrm{F} T})_{i_2} \cdots (\boldsymbol{a}^\dagger e^{-i\mathsf{M}_\mathrm{F} T})_{i_N} |0\rangle. \tag{A.13}$$

Comparing Eq. (A.12) and (A.13), we obtain

$$e^{-i\mathsf{M}_\mathrm{F} T} = \mathcal{T} e^{-i\int_0^T \mathsf{M}(t)dt}. \tag{A.14}$$

This equation gives M_F from $\mathsf{M}(t)$.

When we consider the limit $L, N \to \infty$, we immediately know that although the norm of the many-body Hamiltonian diverges, the convergence radius of the Floquet Magnus expansion is finite even in this limit if the norm of the matrix $\mathsf{M}(t)$ remains finite.

Appendix B

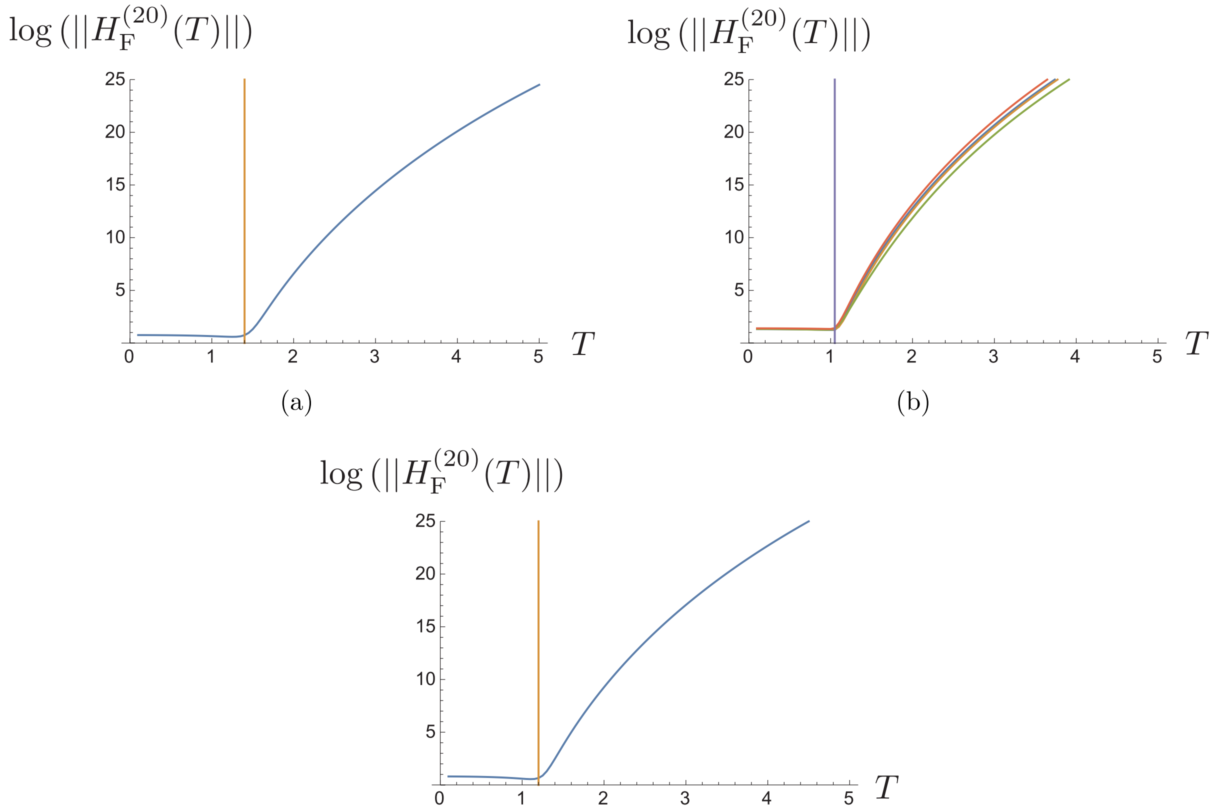
Supplementary numerical results

B.1 Breaking of the convergence of the Floquet-Magnus expansion

In Fig. B.1, we show the magnitude of the effective Hamiltonian obtained by the Floquet-Magnus expansion truncated at 20th order, which we denote as $H_{\mathrm{F}}^{(20)}(T) = \sum_{n=0}^{20} T^n \Omega_n(T)$. We expect this order to be high enough to detect the divergence point of the expansion. The vertical line corresponds to the vertical line in Fig. 1. The figures imply that the Floquet-Magnus expansion is divergent when the driving period is larger than the value indicated by the vertical line.

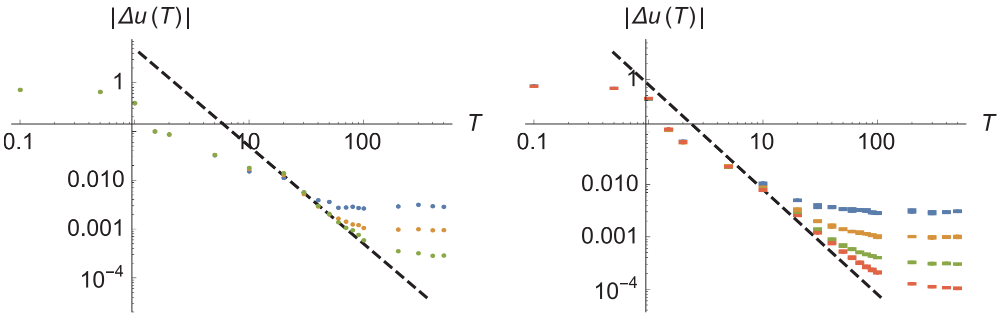
B.2 Energy density difference and the variance of the effective temperatures for the conserved quantities without scaling

In Figs. B.2 and B.3, we show the energy-density difference of the steady state and the variance of $\{\Lambda_p\}_{p=1}^{L}$ against the driving period, respectively. Using these data, we obtained the scaling plots in Fig. 2.



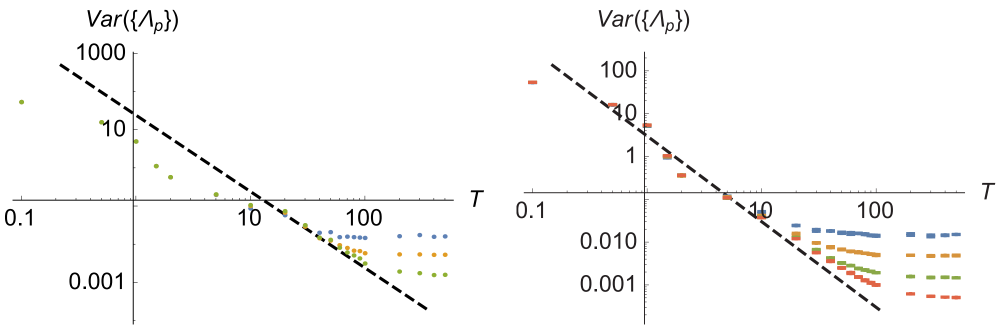
(c)

Figure B.1: Magnitude of $H_{\mathrm{F}}^{(20)}(T)$. We set $\{h_i\}$ in Eq. (8.3) as (a) the quasi-periodic field, (b) the random Gaussian field with four random samples, and (c) the staggered field; see the description below Eq. (8.3). The system size is $L = 500$. The vertical line denotes the driving period where we detected the breaking of the convergence of the expansion.



(a) (b)

Figure B.2: Absolute values of the energy-density difference of the steady state. We set $\{h_i\}$ in Eq. (8.3) as (a) the quasi-periodic fields and (b) the random Gaussian field with four random samples. The driving periods for the data points are T = 0.1, 0.5, 1, 1.5, 2, 5, 10, 20, 30, 40, 50, 60, 70, 80, 90, 100, 200, 300, 400, 500. The system sizes are the same as in Fig. 8.2 of the main text. The larger the system size, the lower lie the data points for large T. (Different colors also indicate different system sizes.) The broken line indicates the behavior T^{-2}.



(a) (b)

Figure B.3: Variance of $\{\Lambda_p\}_{p=1}^{L}$. We set $\{h_i\}$ in Eq. (8.3) as (a) the quasi-periodic fields and (b) the random Gaussian field with four random samples. The driving periods and the system sizes for the data points are the same as those in Fig. B.2. The larger the system size, the lower lie the data points for large T. (Different colors also indicate different system sizes.) The broken line indicates the behavior T^{-2}.

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