Thermalization in Open Many-Body Systems Based on Eigenstate Thermalization Hypothesis

Tatsuhiko Shirai*
Institute for Solid State Physics, University of Tokyo, Kashiwa 5-1-5, Chiba 277-8581, Japan

Takashi Mori†
RIKEN Center for Emergent Matter Science (CEMS), Wako 351-0198, Japan

We investigate steady states of macroscopic quantum systems under dissipation not obeying the detailed balance condition. We argue that the Gibbs state at effective temperature gives a good description of the steady states provided that the system Hamiltonian satisfies the eigenstate thermalization hypothesis (ETH) and the perturbation theory in the weak system-environment coupling is valid in the thermodynamic limit. We numerically show the validity of the perturbation theory in some open quantum systems in spite of the fact that the convergence radius of the perturbation series shrinks to zero in the thermodynamic limit. It is also shown that our theory is not applicable to transport phenomena, in which stationary current of a conserved quantity exists, due to the failure of the perturbation theory. This work suggests a connection between steady states of macroscopic open quantum systems and the ETH.

Introduction.— When a quantum system is weakly coupled to a large environment, it usually relaxes to a steady state due to dissipation [1–3]. When the environment is in thermal equilibrium, the steady state is universally described by the Gibbs state by virtue of the detailed balance condition [4]. In contrast, when the environment is out of equilibrium, the detailed balance condition is violated and there is no simple criterion to determine the steady state. It is a challenge in statistical physics to predict the steady state in such a nonequilibrium situation [5–13].

Recent experimental progress using ultracold atoms and trapped ions has enabled us to introduce controlled dissipation [14–17], which leads us to the possibility of designing dissipation so that the steady state has desired properties [18, 19]. This experimental background also motivates us to theoretically study steady states of quantum systems under dissipation not obeying the detailed balance condition.

In this Letter, the steady state of a quantum many-body system in a weak contact with an out-of-equilibrium environment is investigated. It turns out that the Gibbs state at a certain effective temperature well describes the steady state in some open quantum systems despite the violation of the detailed balance condition. We theoretically argue that there are two ingredients in the realization of a Gibbs steady state, i.e., the validity of the perturbation theory in weak dissipation (i.e., weak system-environment coupling) and the eigenstate thermalization hypothesis (ETH).

As for the weak-dissipation perturbation theory, it is known that its convergence radius vanishes in the thermodynamic limit for generic open quantum systems [20, 21]. Nevertheless, our numerical calculations for spin systems suggest that the leading-order truncation of the perturbative expansion well describes the steady state in the thermodynamic limit provided that no stationary current of a conserved quantity exists. This finding implies that the weak-dissipation perturbative expansion is a kind of an asymptotic expansion. While, it is also shown that the perturbation theory completely fails when there is a stationary current in the bulk, which is a typical situation when two or more reservoirs are coupled to the system. We later demonstrate the failure of the perturbation theory for a one-dimensional Bose-Hubbard model that is coupled to two reservoirs with different chemical potentials at each end.

As for the ETH, it is recognized as an important property of the Hamiltonian in explaining the approach to thermal equilibrium in isolated quantum systems [22–25]. According to the ETH, if a density matrix is diagonal in the basis of energy eigenstates and has a subextensive energy fluctuation, it is indistinguishable from the Gibbs state at a certain effective temperature as far as we look at local observables. As we will see below, in an open quantum system, the leading-order perturbation theory yields a steady state that meets the condition mentioned above. Therefore, by combining the ETH with the perturbation theory, we can conclude that the steady state is described by the Gibbs state irrespective of the detailed balance condition.

In this way, this work suggests a connection between steady states of macroscopic open quantum systems and the ETH. In a recent work [26], it was shown that a Gibbs state with a time-dependent temperature emerges in the transient dynamics of an open quantum system in which the system of interest is finite and obeys the ETH. Our result should be distinguished from this recent result since we here focus on the steady state (i.e., the long-time limit) in a macroscopic open quantum system (i.e., the thermodynamic limit).

Perturbative expansion and ETH.— We consider a macroscopic system of the volume $V$ in contact with an environmental system. We denote by $\rho$ the reduced density matrix of the system of interest, which is assumed to obey the Lindblad equation [1, 27]

$$
\frac{d\rho}{dt} = -i[H, \rho] + \gamma \sum_a \left[ L_a \rho L_a^\dagger - \frac{1}{2} L_a^\dagger L_a \rho \right]
$$

(1)

where $[\cdot, \cdot]$ and $\{\cdot, \cdot\}$ denote the commutator and the anti-commutator, respectively, and we put $\hbar = 1$. The system Hamiltonian is denoted by $H$, and dissipation is characterized by the Lindblad operators $\{L_a\}$. In this Letter, we consider the weak dissipation regime, i.e., small $\gamma$. 

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The steady state $\rho_s$ is defined by $\mathcal{L}\rho_s = 0$. Since $\gamma$ is assumed to be small, we perform the perturbative expansion of $\rho_s$ in $\gamma$:

$$\rho_s = \sum_{n=0}^{\infty} \gamma^n \rho_s^{(n)}.$$  (2)

By substituting this expression into $\mathcal{L}\rho_s$ and requiring that it vanishes in each order in $\gamma$, we obtain

$$[H, \rho_s^{(0)}] = 0$$  (3)

for $O(\gamma^0)$, and

$$-i[H, \rho_s^{(1)}] + \sum_a [L_a \rho_s^{(0)} L_a^\dagger - \frac{1}{2} (L_a^\dagger L_a, \rho_s^{(0)})] = 0$$  (4)

for $O(\gamma^1)$. Equation (3) implies that $\rho_s^{(0)}$ is diagonal in the basis of the eigenstates of $H$. Let us denote by $|\phi_i\rangle$ and $E_i$ the $i$th eigenstate of $H$ and its eigenvalue, respectively. Then, the diagonal part of Eq. (4) reads

$$\sum_i (W_{ij} P_j - W_{ji} P_i) = 0$$  (5)

for every $i$, where $P_i = \langle \phi_i | \rho_s^{(0)} | \phi_i \rangle$ and $W_{ij} = \sum_a | \langle \phi_i | L_a | \phi_j \rangle |^2$. The diagonal elements of $\rho_s^{(0)}$ are determined by the set of equations (5). Here, $W_{ij}$ can be interpreted as the transition probability from the state $j$ to $i$. The transition probabilities satisfy the detailed balance condition

$$W_{ij} = e^{-\beta E_i - E_j}$$  (6)

when the environment is in thermal equilibrium at the inverse temperature $\beta$ [4, 28, 29]. As a result, the steady state is given by the Gibbs state $P_i = e^{-\beta E_i} / Z(\beta)$ with the partition function $Z(\beta) = \sum_i e^{-\beta E_i}$.

When the environment is out of equilibrium, the detailed balance condition is violated, and hence $\{P_i\}$ is not necessarily of the Gibbs form. Nevertheless, we point out that $\rho_s^{(0)}$ is indistinguishable from the Gibbs state if the system Hamiltonian $H$ obeys the ETH. The ETH states that every energy eigenstate $|\phi_i\rangle$ looks thermal in the sense that

$$\langle \phi_i | O | \phi_i \rangle \approx Tr O \frac{e^{-\beta H}}{Z(\beta)}$$  (7)

for any local operator $O$, where $\beta_i$ depends on $i$ through the condition $\langle \phi_i | H | \phi_i \rangle = Tr H e^{-\beta_i H} / Z(\beta_i)$. Since $\beta_i$ is almost constant, $\beta_i \approx \beta$, as long as the energy fluctuation in $\rho_s^{(0)}$ is subextensive, we have

$$Tr O \rho_s^{(0)} \approx Tr O \frac{e^{-\beta H}}{Z(\beta)}.$$  (8)

In this way, the steady state is well described by the Gibbs state for small $\gamma$ as long as the naive perturbation theory is valid.

Validity of perturbation theory.— In Ref. [21], it is numerically shown that the convergence radius of the perturbative expansion of Eq. (2) shrinks to zero in the thermodynamic limit, $V \to \infty$. This means that it is a nontrivial issue whether the thermodynamic limit commutes with the weak-dissipation limit. If they are commutable in evaluating the expectation value of an operator $O$, we have

$$\lim_{\gamma \to 0} \lim_{V \to \infty} Tr O \rho_s = \lim_{V \to \infty} \lim_{\gamma \to 0} Tr O \rho_s = \lim_{V \to \infty} Tr O \rho_s^{(0)}.$$  (9)

For macroscopic systems, the thermodynamic limit should be taken before the weak-dissipation limit, and hence, the left-hand side of Eq. (9) is a quantity what we want. On the other hand, the most right-hand side of Eq. (9) corresponds to the solution in the leading-order perturbation theory.

In this Letter, we consider the relative entropy density between $\rho_s$ and $\rho_s^{(0)}$

$$d \equiv \frac{1}{V} Tr (\rho_s (\ln \rho_s - \ln \rho_s^{(0)}))$$  (10)

If $\lim_{\gamma \to 0} \lim_{V \to \infty} d = 0$, we can conclude the macrostate equivalence between $\rho_s$ and $\rho_s^{(0)}$ [30], i.e., Eq. (9) holds for intensive macroscopic observables $O$ that obey the large-deviation principle in the steady state [31].

Result.— We consider the dissipative Ising chain that is described by Eq. (1) with

$$\begin{cases}
H = \sum_{i=1}^{V} (\Delta S_i^z + \Omega S_i^x + g S_i^x S_{i+1}^z), \\
L_i = S_i^z \text{ for } i = 1, \ldots, V,
\end{cases}$$  (11)

where $\{S_i^z\}_{i=1}^{V}$ are spin-1/2 operators and $S_i^\pm \equiv S_i^x \pm i S_i^y$. The periodic boundary condition is imposed, $S_{V+1}^z = \bar{S}_1^z$. The parameters of the Hamiltonian are set as $(\Delta, \Omega, \gamma) = (1.089, 1.618, 4)$, with which the ETH has been numerically shown to hold [32]. This open quantum system has been implemented using Rydberg atoms [33, 34] and non-equilibrium phase transitions have been theoretically discussed [35]. In this system the up and down spin states correspond to the Rydberg state and the ground state of an atom, respectively, and $\{L_i\}$ describes the spontaneous emission in each atom. It is noted that the detailed balance condition is not satisfied in this model.

We show the system-size dependence of $d$ [Fig. 1] at $\gamma = 0.01, 0.03$ and 0.05 for $4 \leq V \leq 14$. In the figure, we find the linear dependence of the distances on $1/V$ for large $V$ ($V \geq 9$). By using this linear dependence, we extrapolate the data for each $\gamma$ to the thermodynamic limit. In this way we calculate $\lim_{V \to \infty} d$ for several small values of $\gamma$, which are presented in Fig. 2. We find that for $\gamma \leq 0.02$,

$$\lim_{V \to \infty} d \propto \gamma,$$  (12)

showing that the distance approaches zero in the limit of $\gamma \to 0$. 

is not always the case. We now argue that the perturbation theory fails for open quantum systems whose steady state has conserved currents in the bulk.

As an example, suppose a one-dimensional system in contact with two particle reservoirs with different chemical potentials at each end. The chemical potential difference drives the system, and particles will flow in the bulk. In the steady state, the local chemical potential will have a gradient, which results in a non-uniform particle density profile. On the other hand, if the system Hamiltonian possesses the translation invariance in the bulk, an individual energy eigenstate shows a uniform density profile, and hence its mixture like \( \rho_s^{(0)} \) cannot reproduce the expected non-uniform density profile in the steady state. This argument can be generalized to other conserved currents (e.g., an energy current between two thermal reservoirs at different temperatures). The perturbation theory fails in such a situation.

We now demonstrate the failure of the perturbation theory in the hard-core Bose-Hubbard model driven by two environments with different chemical potentials:

\[
H = - \sum_{i=1}^{V-1} h(b_i b_{i+1}^\dagger + b_i^\dagger b_{i+1}) + J n_i n_{i+1} \\
- \sum_{i=1}^{V-2} h'(b_{i+1} b_{i+2}^\dagger + b_{i+2}^\dagger b_{i+1}) + J' n_i n_{i+2},
\]

(14)

where \( b_i \) and \( b_i^\dagger \) are annihilation and creation operators of a boson at site \( i \), and \( n_i = b_i^\dagger b_i = 0 \) or 1. The parameters of Hamiltonian are given by \( (h, h', J, J') = (0.9167, 0.2449, 4, 0.9045) \). The Lindblad operators \( \{L_\alpha\}_{\alpha=1}^4 \) act on the boundaries of the lattice and \( \mu \) effectively controls the chemical potential of the environments. We set \( \mu = 0.1 \).

A typical particle number profile in the steady state is shown in Fig. 4. A non-uniform profile is observed. The system-size dependences of \( d \) at \( \gamma = 0.01, 0.03 \) and 0.05 are shown in Fig. 5. Again, we find linear dependence on \( 1/V \), so the value in the thermodynamic limit is estimated by extrapolating the
data. In this way, we obtain the $\gamma$-dependence of $\lim_{V \to \infty} d$ [Fig. 6], showing that the distance is finite in the limit of $\gamma \to 0$:

$$\lim_{\gamma \to 0} \lim_{V \to \infty} d \neq 0.$$  \hspace{1cm} (15)

This result clearly shows that the perturbation theory fails in the thermodynamic limit when there is a conserved current in the steady state.

Summary.—In this Letter, we have investigated steady states of macroscopic quantum systems under dissipation not obeying the detailed balance condition. We have theoretically argued that even in such non-equilibrium situations, the Gibbs state at effective temperature is a good description of the steady states. There are two ingredients in emergence of the Gibbs state: the validity of the weak-dissipation perturbation theory and the ETH. In spite of the fact that the convergence radius of the weak-dissipation expansion generically tends to zero in the thermodynamic limit [20, 21], our numerical results suggest that this expansion is an asymptotic expansion, and thus its leading-order truncation well describes the steady state, if there is no stationary current of a conserved quantity. By applying the ETH, we have concluded that the steady state is given by the Gibbs state. We emphasize that our theory is not applicable to transport phenomena; the steady state deviates from the Gibbs state when there is a stationary current in the bulk, due to the failure of the perturbation theory.

There remain some issues to be studied. Our result implies that the weak-dissipation expansion is an asymptotic expansion with the zero convergence radius in the thermodynamic limit, but its rigorous proof is missing. The effect of extensive number of conserved quantities in integrable models on the steady states and the extension of our theory to systems with finite dissipation strength are also important open problems.

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* shirai@exa.phys.s.u-tokyo.ac.jp
† takashi.mori.fh@riken.jp

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Supplemental Materials

Tatsuhiko Shirai and Takashi Mori
Institute for Solid State Physics, University of Tokyo, Kashiwa 5-1-5, Chiba 277-8581, Japan
RIKEN Center for Emergent Matter Science (CEMS), Wako 351-0198, Japan

A. CONVERGENCE RADIUS OF PERTURBATIVE SERIES

Lemos and Prosen [21] developed the numerical method to estimate the convergence radius of the perturbative expansion, \( \gamma_c \), and they argued that \( \gamma_c \) shrinks to zero with the system size for generic open quantum systems. In the main text, we have performed the linear fitting of the numerical data for large system size at different values of \( \gamma \) to obtain \( \lim_{V \to \infty} d \). In the argument, we have assumed that \( \gamma = 0.005 \) is greater than \( \gamma_c \) for \( V = 9 \). Here, we show that it is true for our model [Eq. (11)].

In Fig. 7(a), the system-size dependence of \( \gamma_c \) is presented up to \( V = 5 \). The convergence radius \( \gamma_c \) shows the exponential decay with the system size, and it suggests that \( \gamma_c \) shrinks to zero in the thermodynamic limit. However, as in Ref. [21] we could not obtain \( \gamma_c \) for larger system size.

In order to estimate \( \gamma_c \) for larger system size \( (V \geq 6) \), we compare two perturbative solutions, which are obtained by truncation of the perturbation series [Eq. (2)] up to 4th order and 6th order. In Fig. 7(b), we plot the expectation values of \( \sum_{i=1}^{V} S^x_i / V \) over each perturbative solution by solid curve (4th order) and dotted curve (6th order), respectively. We found that two curves start to deviate at a certain value of \( \gamma \), and the value is close to \( \gamma_c \) for \( V = 5 \). We use this relation to estimate the approximated values of \( \gamma_c \) for larger system size. In Fig. 7(b), we found the approximated value of \( \gamma_c \) decreases with the system size and it is smaller than 0.005 for \( V = 9 \).
B. EMERGENCE OF THE GIBBS STATE IN ANOTHER DISSIPATIVE SPIN SYSTEM

We provide another dissipative model that shows the same $\gamma$-dependence of $\lim_{V \to \infty} d$ as the model in the main text. The Hamiltonian and the Lindblad operators are given by

\[
\begin{align*}
H &= \sum_{i=1}^{V} \left( \Delta S_i^z + \Omega S_i^z S_{i+1}^z + g S_i^z S_{i+1}^z + g' S_i^z S_{i+2}^z \right), \\
L_i &= S_i^- \text{ for } i = 1, \cdots, V,
\end{align*}
\]

where $(\Delta, \Omega, g, g') = (-1.809, 3.236, -4, -2)$.

In Fig. 8, we show the system-size dependences of $d$ at $\gamma = 0.01, 0.03, \text{ and } 0.05$. We find the linear dependence of the distance on $1/V$ for large $V$ ($V \geq 9$), and again we extrapolate the data for each $\gamma$ to the thermodynamic limit. In Fig. 9, we present $\lim_{V \to \infty} d$ as a function of $\gamma$. The figure shows $\lim_{V \to \infty} d \propto \gamma$, which are the same dependence as the model of the main text.

![FIG. 8. System-size dependence of $d$ for the dissipative model [Eq. (B.1)], in which no stationary current exists in the steady state. Points are numerical data: $\gamma = 0.01$(circle) $0.03$(triangle), and $0.05$(square). The data for each $\gamma$ shows linear dependence on $1/V$ for large $V(V \geq 9)$.](image)

![FIG. 9. $\gamma$-dependence of $\lim_{V \to \infty} d$. Full curve is a guide to show the dependence for small $\gamma (\gamma \leq 0.05)$, $\lim_{V \to \infty} d \propto \gamma$.](image)