Microscopic analysis of the microscopic reversibility in quantum systems

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Abstract. We investigate the robustness of the microscopic reversibility in open quantum systems which is discussed by Monnai in a recent article. We derive an exact relation between the forward transition probability and the reversed transition probability in the case of a general measurement basis. We show that the microscopic reversibility acquires some corrections in general and discuss the physical meaning of the corrections. Under certain processes, some of the correction terms vanish and we numerically confirmed that the remaining correction term becomes negligible; for such processes, the microscopic reversibility almost holds even when the local system cannot be regarded as macroscopic.

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1. Introduction

Understanding of non-equilibrium quantum dynamics has been eagerly pursued since many experiments are done under non-equilibrium situations and should also be treated quantum mechanically. While there are many physical quantities and relations to characterize the properties of the equilibrium systems, very few are known for the systems out of equilibrium. The linear response theory, which describes the non-equilibrium quantities in terms of the equilibrium quantities, is a powerful tool to investigate such systems. It is, however, restricted to the case where the systems are close to equilibrium. In order to describe the behavior of strongly non-equilibrium systems, it may be required to find some relations which contain detailed information of the dynamics.

For exploring the character of the strongly non-equilibrium dynamics of quantum systems, symmetry relations for non-equilibrium states such as fluctuation theorems are of great importance [1]–[9]. In particular, significant attention is paid to the relation between the transition probabilities of forward processes and the transition probabilities of the corresponding reversed processes [2, 3], [5]–[9]. Such relations are appealing particularly because they are not restricted to the close-to-equilibrium states. As the forward process of the fluctuation theorems, it is typical to consider a driven system which is in the thermal equilibrium state at \( t = 0 \) and then is controlled by a time-dependent external parameter \( \lambda(t) \). We consider the case where the states at the beginning and the ending of the process are measured, and thus the states are projected. We can interpret that the state hopped from the one to the other; the transition probability of the forward process is defined as the probability that such a transition occurs. For the reversed process, it is common to consider the following in quantum systems [2, 3, 5, 8, 9]. (See [10]–[13] for discussions...
in classical systems.) The initial density matrix of the reversed process is set to be the same as that of the forward process but with the value of the external parameter $\lambda(T)$, where $T$ is the final moment of the forward process. Then, the system is driven with a time-reversed protocol $\lambda(T-t)$; the transition probability of the reversed process is defined as the probability that the opposite transition occurs compared to the transition of the forward process.

They are the typical settings for the study of fluctuation theorems. From the viewpoint of quantum operation, however, it may be natural to set the time-evolved (generally non-equilibrium) state as the initial density matrix of the reversed process.

As another point for the study of open quantum systems, the choice of the measurement process is especially significant; measurement processes on a reservoir [4] or both on a local system and a reservoir [2, 3, 5, 8] are often considered. Nevertheless, sometimes it is more natural to consider the measurement solely on the local system; in the present paper, we consider such a case. There are fluctuation theorems of open quantum systems which are written solely in the terms of the local system though they do not take into account the measurement process in order to discuss the forward and the reversed processes [14, 15].

The above two points were taken into account in a recent study by Monnai [16]. The study pointed out the significance of the microscopic reversibility in open quantum systems as a kind of symmetry relation similar to, but different from, the fluctuation theorems [16]. It defines the reversed process as the one from the time-evolved state and considers the measurements on the local system only.

The discussion in [16] for open quantum systems is as follows. The total Hamiltonian consists of the Hamiltonian of a local system $\hat{H}_s(\lambda(t))$ which is controlled by external forces with the parameter $\lambda(t)$, the Hamiltonian of a reservoir $\hat{H}_r$ and the Hamiltonian of coupling between them $\hat{H}_c$, i.e.

$$\hat{H}_{\text{tot}}(t) = \hat{H}_s(\lambda(t)) + \hat{H}_r + \hat{H}_c. \quad (1)$$

Let us consider the process where we measure the states of the local system at $t=0$ and $T$. Throughout this paper, we employ the Schrödinger picture and only consider the projection measurement as the measurement protocol. The measurement basis at $t=0$ can be different from the one at $t=T$. We refer to the measured states as $|n(0)\rangle$ and $|m(T)\rangle$ and to the probability of such a transition as $p_F(|n(0)\rangle \rightarrow |m(T)\rangle)$. Note that the time variables of $|n(0)\rangle$ and $|m(T)\rangle$ merely indicate the moments that the measurements are done along the forward process; they do not mean that those measurement bases are time-dependent. Next, the reversed process is defined as follows; as the initial state, we prepare the state $\hat{\rho}(T)$ that evolved from $t=0$ to $T$ without the measurement at $t=0$, and then drive the system from $t=T$ to $2T$ with the time-reversed protocol $\lambda(2T-t)$. The reversed transition probability is defined to be the probability of observing $\Theta|m(T)\rangle$ at $t=T$ and $\Theta|n(0)\rangle$ at $t=2T$ under the time-reversed process, where $\Theta$ is the time-reversal operator. We refer to such a transition probability as $p_R(\Theta|m(T)\rangle \rightarrow \Theta|n(0)\rangle)$. Monnai then showed the equality [16]

$$p_F(|n(0)\rangle \rightarrow |m(T)\rangle) = p_R(\Theta|m(T)\rangle \rightarrow \Theta|n(0)\rangle) \quad (2)$$

under the following conditions: (i) the total system is a product state at $t=0$; (ii) the local system is macroscopic, so that the contribution from the coupling Hamiltonian $\hat{H}_c$ is
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extremely small compared to the ones from the local system $\hat{H}_x$ and the reservoir $\hat{H}_r$, and we thereby have $U(T)(\sqrt{\rho_x(0)} \otimes \sqrt{\rho_r(0)})U^\dagger(T) \simeq \sqrt{\rho_x(T)} \otimes \sqrt{\rho_r(0)}$, where $\rho_x$ and $\rho_r$ are the density matrices of the local system and the reservoir, respectively; and (iii) the measured states at $t = 0$ and $T$ are the eigenstates of the density matrix of the local system. We call the equality (2) the microscopic reversibility in open quantum systems. Note that it is a relation about the local system; no measurements are done on the reservoir.

The main purpose of this paper is to investigate the robustness of the microscopic reversibility (2). Although we assume that the initial state is a product state, we will allow the final state to be arbitrary; we will not assume the local system to be macroscopic and we will consider an arbitrary measurement bases. We will also assume that $\langle m(T)|\hat{\Theta}|\hat{\rho}(T)\hat{\Theta}|m(0)\rangle = \langle m(T)|\hat{\rho}(T)|m(0)\rangle$; the probability to obtain the resulting state $|m(T)\rangle$ is equal to that of the time-reversed state. As a result, we will show that the microscopic reversibility does not hold exactly in general; it acquires correction terms. The origin of the corrections is the effect that the measurement processes destroy the quantum coherence of the system that we measure. Although the microscopic reversibility is broken in general, if we measure the eigenstate of the density matrix of the local system at $t = 0$, the form of the correction becomes very simple. In the case of a thermal relaxation process, we numerically confirmed that the correction term is small enough compared to the forward and the reversed transition probabilities in open quantum systems.

This paper is organized as follows: in section 2, we will derive the microscopic reversibility in isolated quantum systems with correction terms under general measurement bases. As a simple example, we will consider the case of a free particle; we will show that a correction term can be very large in this case, and thus we cannot see the microscopic reversibility at all. In section 3, we will derive the microscopic reversibility of open systems with correction terms. If the initial and the final states are product states and the eigenstates of the density matrices of the local system are measured, we will show that the correction terms vanish and the microscopic reversibility holds exactly. We will also show that, if we disconnect the local system from the reservoir, the correction term then becomes constant. In section 4, we analyze the details of the corrections. Finally, in section 5, we numerically compute a correction to the microscopic reversibility for a one-dimensional spin chain; we regard the first two spins as the local system and the rest as the reservoir. The result shows that the correction is relatively small, so that the microscopic reversibility almost holds even when the local system cannot be regarded as macroscopic.

2. Microscopic reversibility in isolated systems

We first describe the microscopic reversibility in isolated quantum systems with the same notations and processes as in section 1. The forward and the reversed transition probabilities are [1]

$$p_F(|m(0)\rangle \rightarrow |m(T)\rangle) = \langle m(T)|\hat{U}|n(0)\rangle \langle n(0)|\hat{\rho}(0)|n(0)\rangle \langle n(0)|\hat{U}^\dagger|m(T)\rangle,$$

(3)

$$p_R(\hat{\Theta}|m(T)\rangle \rightarrow \hat{\Theta}|n(0)\rangle) = \langle n(0)|\hat{U}^\dagger|m(T)\rangle \langle m(T)|\hat{\Theta}\hat{\rho}(T)\hat{\Theta}|m(T)\rangle \langle m(T)|\hat{U}|n(0)\rangle.$$ 

(4)

Throughout this paper, we consider the case where $\langle m(T)|\hat{\Theta}\hat{\rho}(T)\hat{\Theta}|m(T)\rangle = \langle m(T)|\hat{\rho}(T)|m(T)\rangle$. This condition is satisfied, for example, in the case where the states

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from a different viewpoint, let us derive the relation between

\[ p_F(|n(0)\rangle \rightarrow |m(T)\rangle) = f_{nm}(T, 0) p_R(\hat{\Theta}|m(T)\rangle \rightarrow \hat{\Theta}|n(0)\rangle), \]  

where \( f_{nm}(T, 0) = \langle n(0)|\hat{\rho}(0)|n(0)\rangle / \langle m(T)|\hat{\rho}(T)|m(T)\rangle \). Let us consider the trivial case where we choose the measurement bases at \( t = 0 \) and \( T \) as the eigenstates of the density matrices \( \hat{\rho}(0) \) and \( \hat{\rho}(T) \), respectively. If we denote \( |n'(T)\rangle := U|n(0)\rangle \), we have \( \langle m(T)|U|n(0)\rangle = \delta_{n'm} \) and therefore

\[ \langle n(0)|\hat{\rho}(0)|n(0)\rangle = \langle n(0)|U^\dagger \hat{\rho}(0)U^\dagger U|n(0)\rangle = \delta_{n'm}\langle m(T)|\hat{\rho}(T)|m(T)\rangle. \]  

Hence the microscopic reversibility trivially holds:

\[ p_F(|n(0)\rangle \rightarrow |m(T)\rangle) = p_R(\hat{\Theta}|m(T)\rangle \rightarrow \hat{\Theta}|n(0)\rangle). \]  

In many cases, however, it is difficult to detect the eigenstates of an arbitrary density matrix or make the system have a density matrix whose eigenstates coincide with the measurement basis that we choose. In the case where the measurement basis is not the eigenstates of the density matrix, we have \( f_{nm}(T, 0) \neq \delta_{n'm} \).

In order to observe the effect of the measurement on the microscopic reversibility from a different viewpoint, let us derive the relation between \( p_F(|n(0)\rangle \rightarrow |m(T)\rangle) \) and \( p_R(\hat{\Theta}|m(T)\rangle \rightarrow \hat{\Theta}|n(0)\rangle) \) in the operator-sum representation [17]. The forward and the reversed transition probabilities are, instead of equations (3) and (4), expressed as

\[ p_F(|n(0)\rangle \rightarrow |m(T)\rangle) = \text{Tr} \hat{P}_n U \hat{P}_n \hat{\rho}(0) \hat{P}_n U^\dagger \hat{P}_m, \]  

\[ p_R(\hat{\Theta}|m(T)\rangle \rightarrow \hat{\Theta}|n(0)\rangle) = \text{Tr} \hat{P}_m U^\dagger \hat{P}_m \hat{\rho}(T) \hat{P}_m U \hat{P}_n, \]

where \( \hat{P}_n = |n(0)\rangle \langle n(0)| \) and \( \hat{P}_m = |m(T)\rangle \langle m(T)| \). Introducing the complementary operator \( \hat{Q}_n \) and \( \hat{Q}_m \) of \( \hat{P}_n \) and \( \hat{P}_m \), i.e.

\[ \hat{Q}_k \equiv \hat{I} - \hat{P}_k, \quad \hat{P}_k \hat{Q}_k = 0, \quad (k = n, m) \]

we can transform the forward transition probability as follows:

\[
p_F(|n(0)\rangle \rightarrow |m(T)\rangle) = \text{Tr} \hat{U}^\dagger \hat{P}_m U \hat{P}_n \hat{\rho}(0) \hat{P}_n = \text{Tr} \hat{U}^\dagger \hat{P}_m \hat{\rho}(T)(\hat{P}_m + \hat{Q}_m) \hat{U}^\dagger \hat{\rho}^{-1}(0) \hat{P}_n \hat{\rho}(0) \hat{P}_n \]

\[ + \text{Tr} \hat{U}^\dagger \hat{P}_m \hat{\rho}(T) \hat{Q}_m \hat{U}^\dagger \hat{\rho}^{-1}(0) \hat{P}_n \hat{\rho}(0) \hat{P}_n \]

\[
= \text{Tr} \hat{U}^\dagger \hat{P}_m \hat{\rho}(T) \hat{P}_m \hat{\rho}^{-1}(0) \hat{P}_n \hat{\rho}(0) \hat{P}_n + \text{Tr} \hat{U}^\dagger \hat{P}_m \hat{\rho}(T) \hat{Q}_m \hat{U}^\dagger \hat{\rho}^{-1}(0) \hat{P}_n \hat{\rho}(0) \hat{P}_n \]

\[ + \text{Tr} \hat{U}^\dagger \hat{P}_m \hat{\rho}(T) \hat{P}_m \hat{\rho}^{-1}(0) \hat{P}_n \hat{\rho}(0) \hat{P}_n. \]

Therefore, we have

\[
\frac{p_F(|n(0)\rangle \rightarrow |m(T)\rangle)}{p_R(\hat{\Theta}|m(T)\rangle \rightarrow \hat{\Theta}|n(0)\rangle)} = g_n + \xi, \]

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where

\[ g_n \equiv \langle n(0)|\hat{\rho}^{-1}(0)|n(0)\rangle \langle n(0)|\hat{\rho}(0)|n(0)\rangle, \]

\[ \xi \equiv \frac{\text{Tr} \hat{U}^\dagger \hat{P}_m \hat{\rho}(T) \hat{Q}_m \hat{U} \hat{\rho}^{-1}(0) \hat{P}_n \hat{\rho}(0) \hat{P}_n + \text{Tr} \hat{U}^\dagger \hat{P}_n \hat{\rho}(T) \hat{P}_m \hat{U} \hat{Q}_n \hat{\rho}^{-1}(0) \hat{P}_n \hat{\rho}(0) \hat{P}_n}{p_R(\Theta|m(T)\rangle \rightarrow \hat{\Theta}|n(0)\rangle). \]  

(14)

We assumed that \( \hat{\rho}(0) \) is the state where its inverse exists. In order to see the structure of the correction term \( \xi \) more explicitly, let us divide it in the following way:

\[ \xi = p_R^{-1} \text{Tr} \hat{U}^\dagger \hat{P}_m \hat{\rho}(T)(\hat{Q}_m \hat{U} + \hat{P}_m \hat{U} \hat{Q}_n)\hat{\rho}^{-1}(0) \hat{P}_n \hat{\rho}(0) \hat{P}_n \]

\[ = p_R^{-1} \text{Tr} \hat{U}^\dagger \hat{P}_m \hat{\rho}(T)[\hat{Q}_m \hat{U}(\hat{P}_n + \hat{Q}_n) + \hat{P}_m \hat{U} \hat{Q}_n]\hat{\rho}^{-1}(0) \hat{P}_n \hat{\rho}(0) \hat{P}_n \]

\[ = p_R^{-1} g_n \text{Tr} \hat{U}^\dagger \hat{P}_m \hat{\rho}(T)\hat{Q}_m \hat{U} \hat{P}_n + \text{Tr} \hat{U}^\dagger \hat{P}_m \hat{\rho}(T)\hat{U} \hat{Q}_n \hat{\rho}^{-1}(0) \hat{P}_n \hat{\rho}(0) \hat{P}_n \]

\[ =: \xi_\alpha + \xi_\beta. \]  

(15)

As a special case, let us consider the situation where we measure the density matrix at \( t = 0 \) with the eigenstate basis and obtain the result \( |n(0)\rangle \), i.e. \( \hat{\rho}(0) \hat{P}_n = p_n \hat{P}_n \) and \( \hat{\rho}^{-1}(0) \hat{P}_n = p_n^{-1} \hat{P}_n \), where \( p_n \) is an eigenvalue of the density matrix \( \hat{\rho}(0) \) for \( |n(0)\rangle \). Then we have \( g_n = p_n p_n^{-1} = 1 \) and \( \xi_\beta = 0 \), but \( \xi_\alpha \neq 0 \in \mathbb{R} \):

\[ \frac{p_R(|n(0)\rangle \rightarrow |m(T)\rangle)}{p_R(\Theta|m(T)\rangle \rightarrow \hat{\Theta}|n(0)\rangle)} = 1 + \xi_\alpha, \]

(16)

where

\[ \xi_\alpha = p_R^{-1} \text{Tr} \hat{U}^\dagger \hat{P}_m \hat{\rho}(T)\hat{Q}_m \hat{U} \hat{P}_n. \]  

(17)

Using (5), we can relate the correction term \( \xi_\alpha \) to \( f_{nm}(T,0) \) as

\[ f_{nm}(T,0) = 1 + \xi_\alpha. \]  

(18)

When we measure the eigenstate of the density matrix at \( t = T \), on the other hand, we have \( \xi_\alpha = 0 \). As we will explain in detail in section 4 for open systems, the corrections \( g_n, \xi_\alpha \) and \( \xi_\beta \) depend on the choices of the measurement bases and, in the case of an open system, on the state of the total system as well. We can use \( g_n, \xi_\alpha \) and \( \xi_\alpha \) as the measures of the irreversibility caused by the measurement processes. The analysis of (12) is more advantageous than (5) in the case of open quantum systems as we will see in section 3.

2.1. Example: one-dimensional free particle

A free particle in one dimension is the simplest illustrative example. We assume that the initial state is given by

\[ \hat{\rho}(0) = \frac{1}{2}|\phi_1(0)\rangle \langle \phi_1(0)| + \frac{1}{2}|\phi_2(0)\rangle \langle \phi_2(0)|, \]  

(19)

where \( |\phi_k(0)\rangle \) \( (k = 1,2) \) are the Gaussian wavepackets in the position representation:

\[ \langle x|\phi_k(0)\rangle = \frac{1}{(\sqrt{\pi} a^2)^{1/4}} \exp\left(\frac{i p_0^{(k)} x - x^2}{2a^2}\right), \]  

(20)
Figure 1. The $T$ dependence of $\xi_\alpha$ with $p_0^{(1)} = 1$, $p_0^{(2)} = 2$, $M = 1$ and $a = 1.2$.

where $x$ and $p^{(k)}_0$ are the position and the momentum of the particle and the parameter $a$ determines the width of the wavepacket. Denoting $M$ as the mass of the particle, we can write the state at $t = T$ as

$$\hat{\rho}(T) = \frac{1}{2}\langle\phi_1(T)|\phi_1(T)\rangle + \frac{1}{2}\langle\phi_2(T)|\phi_2(T)\rangle,$$

(21)

$$\langle x|\phi_k(T)\rangle = \left[\sqrt{\pi} \left(a + \frac{iT}{Ma}\right)\right]^{-1/2} \exp\left[\left(a + \frac{iT}{Ma}\right)^{-1} a \left(-\frac{x^2}{2a^2} + ip^{(k)}_0 x - \frac{ip^{(k)}_0 a T}{2M}\right)\right].$$

(22)

We measure the initial state with the basis which contains $|\phi_1(0)\rangle$ and $|\phi_2(0)\rangle$ and measure the position $x$ at $t = T$; we have $g_n = 1$ and $\xi_\beta = 0$. For the transition from $\phi_1(0)$ to $x(T)$, we have

$$\langle\phi_1(0)|\hat{\rho}(0)|\phi_1(0)\rangle = \frac{1}{2},$$

$$\langle x(T)|\hat{\rho}(T)|x(T)\rangle = \frac{1}{2}\langle x(T)|\phi_1(T)\rangle^2 + \frac{1}{2}\langle x(T)|\phi_2(T)\rangle^2,$$

$$p_F(|n(0)\rangle \rightarrow |m(T)\rangle) = |\langle x(T)|\hat{U}|\phi_1(0)\rangle|^2 |\langle \phi_1(0)|\hat{\rho}(0)|\phi_1(0)\rangle|^2$$

(23)

$$= \frac{1}{2}\langle x(T)|\phi_1(T)\rangle^2,$$

which, according to (18), gives

$$\xi_\alpha = (|\langle x(T)|\phi_1(T)\rangle|^2 + |\langle x(T)|\phi_2(T)\rangle|^2)^{-1} - 1.$$  

(24)

The $T$ dependences of $\xi_\alpha$ is plotted in figure 1. Here, we set $p_0^{(1)} = 1$, $p_0^{(2)} = 2$, $M = 1$ and $a = 1.2$. The inverse of the correction term $\xi_\alpha^{-1}$ vanishes as $x$ and $T$ increase, which means that the correction grows much larger than unity; we cannot see the microscopic reversibility at all in this example.

For the isolated quantum systems, we confirmed that the microscopic reversibility is not a general relation. Because there is nothing like thermalization, the deviation from
the microscopic reversibility seems to depend sensitively on the choice of the system and the protocol; the microscopic reversibility is not a proper relation to characterize the dynamics of the isolated quantum systems. For the open quantum systems, nevertheless, we expect the microscopic reversibility is indeed a proper relation due to the effect of the thermalization; we will show in section 5 that our expectation seems to be correct.

3. Microscopic reversibility in open quantum systems

We next extend the discussion in section 2 to the case of open quantum systems. Let us consider the microscopic reversibility of the local quantum system which is thrown into a reservoir at \( t = 0 \). We allow the local system and the reservoir to be externally controlled by time-dependent parameters \( \lambda_s(t) \) and \( \lambda_r(t) \). The total Hamiltonian is

\[
\hat{H}_{\text{tot}}(t) = \hat{H}_s(\lambda_s(t)) + \hat{H}_r(\lambda_r(t)) + \hat{H}_c\theta(t),
\]

(25)

where \( \hat{H}_s(\lambda_s(t)) \), \( \hat{H}_r(\lambda_r(t)) \) and \( \hat{H}_c \) are the Hamiltonians of the local system, the reservoir and the coupling between the local system and the reservoir, respectively. The function \( \theta(t) \) is a step function. Since we consider the situation where the coupling is turned on at \( t = 0 \), the initial state is given as a product state

\[
\hat{\rho}_{\text{tot}}(0) = \hat{\rho}_s(0) \otimes \hat{\rho}_r(0).
\]

As we mentioned in section 1, we consider the forward and the reversed transition probabilities of the local system under the constraint that we measure the local system only. The transition probability of the forward process that the state of the local system evolves from \( |n(0)\rangle \) to \( |m(T)\rangle \) is

\[
p_F(|n(0)\rangle \rightarrow |m(T)\rangle) = \text{Tr}\langle m(T)|\hat{U}|n(0)\rangle\langle n(0)|\hat{\rho}_{\text{tot}}(0)|n(0)\rangle\langle n(0)|\hat{U}^\dagger|m(T)\rangle
\]

(27)

and the reversed transition probability that the state of the local system evolves from \( \Theta|m(T)\rangle \) to \( \Theta|n(0)\rangle \) is

\[
p_R(\Theta|m(T)\rangle \rightarrow \hat{\Theta}|n(0)\rangle) = \text{Tr}\langle m(T)|\hat{U}^\dagger|m(T)\rangle\langle m(T)|\hat{\rho}_{\text{tot}}(T)|m(T)\rangle\langle m(T)|\hat{U}|n(0)\rangle,
\]

(28)

where \( \langle m(T)|\hat{U}\rangle|n(0)\rangle \), \( \langle n(0)|\rho_{\text{tot}}(0)|n(0)\rangle \) and \( \langle n(0)|\hat{U}^\dagger|m(T)\rangle \) are the operators on the reservoir, whereas Tr\(_r\) is the trace with respect to the degrees of freedom of the reservoir. As in the case of isolated systems, we again assumed that \( \langle m(T)|\hat{\Theta}\hat{\rho}_{\text{tot}}(T)\hat{\Theta}|m(T)\rangle = \langle m(T)|\hat{\rho}_{\text{tot}}(T)|m(T)\rangle \). Note that \( p_F(|n(0)\rangle \rightarrow |m(T)\rangle) \) is indeed a real number since \( \hat{\rho}_{\text{tot}}(0) \) is Hermitian:

\[
p_F(|n(0)\rangle \rightarrow |m(T)\rangle)^* = \sum_{x,x',y} \langle m(T), y|\hat{U}|n(0), x\rangle\langle n(0), x|\hat{\rho}_{\text{tot}}(0)|n(0), x'\rangle\langle n(0), x'|\hat{U}^\dagger|m(T), y\rangle^*
\]

\[
= \sum_{x,x',y} \langle m(T), y|\hat{U}|n(0), x'\rangle\langle n(0), x'|\hat{\rho}_{\text{tot}}(0)|n(0), x\rangle\langle n(0), x|\hat{U}^\dagger|m(T), y\rangle
\]

\[
= p_F(|n(0)\rangle \rightarrow |m(T)\rangle),
\]

(29)

where \( x, x', \) and \( y \) are the states of the reservoir.
As we did for isolated systems, let us introduce the projection operators $\hat{P}_n$ to project on the state $|n(0)\rangle$ of the local system at time $t = 0$ and $\hat{Q}_n$ to project on the complementary space of $\hat{P}_n$, i.e.

$$\hat{P}_n \equiv \sum_{x(0)} |n(0), x(0)\rangle \langle n(0), x(0)|, \quad \hat{Q}_n \equiv \hat{I} - \hat{P}_n. \quad (30)$$

Similarly, we define $\hat{P}_m$ to project on the state $|m(T)\rangle$ of the local system at time $t = T$ and $\hat{Q}_m$ to project on the complementary space of $\hat{P}_m$, i.e.

$$\hat{P}_m \equiv \sum_{x(T)} |m(T), x(T)\rangle \langle m(T), x(T)|, \quad \hat{Q}_m \equiv \hat{I} - \hat{P}_m. \quad (31)$$

Now, we rewrite the forward probability as follows:

$$p_F(|n(0)\rangle \rightarrow |m(T)\rangle) = \text{Tr} \hat{U} \hat{P}_m \hat{U} \hat{P}_n \rho_{\text{tot}}(0) \hat{P}_n = \text{Tr} \hat{U} \hat{P}_m \rho_{\text{tot}}(0) \hat{U} \hat{P}_n \hat{P}_n = \text{Tr} \hat{U} \hat{P}_m \hat{P}_n \rho_{\text{tot}}(0) \hat{P}_n \hat{P}_n$$

$$= \text{Tr} \hat{U} \hat{P}_m \hat{P}_n \rho_{\text{tot}}(0) \hat{P}_n \hat{P}_n$$

$$+ \text{Tr} \hat{U} \hat{P}_m \hat{P}_n \rho_{\text{tot}}(0) \hat{P}_n \hat{P}_n$$

$$= \text{Tr} \hat{U} \hat{P}_m \hat{P}_n \rho_{\text{tot}}(0) \hat{P}_n \hat{P}_n$$

We assume that the initial state is the product state (26), but the measurement bases are not necessarily the eigenstates of the density matrix of the local system, and thus the first term of equation (32) is

$$\text{Tr} \hat{U} \hat{P}_m \rho_{\text{tot}}(0) \hat{P}_n \rho_{\text{tot}}^{-1}(0) \hat{P}_n \rho_{\text{tot}}(0) \hat{P}_n = g_n p_R(\hat{\Theta}|m(T)\rangle \rightarrow \hat{\Theta}|n(0)\rangle),$$

where

$$g_n \equiv \langle n(0)|\hat{\rho}_s^{-1}(0)|n(0)\rangle \langle n(0)|\hat{\rho}_n(0)|n(0)\rangle. \quad (34)$$

We do exactly the same transform as equation (15) for the second and third terms except that the density matrix is $\hat{\rho}_{\text{tot}}$ and the projection operators are for the local system only. Then we arrive at one of the major results of the present paper:

$$\frac{p_F(|n(0)\rangle \rightarrow |m(T)\rangle)}{p_R(\hat{\Theta}|m(T)\rangle \rightarrow \hat{\Theta}|n(0)\rangle)} = g_n + \xi_\alpha + \xi_\beta,$$

where

$$\xi_\alpha \equiv p_R^{-1} g_n \text{Tr} \hat{U} \hat{P}_m \rho_{\text{tot}}(T) \hat{Q}_m \hat{U} \hat{P}_n,$$

$$\xi_\beta \equiv p_R^{-1} \text{Tr} \hat{U} \hat{P}_m \rho_{\text{tot}}(T) \hat{U} \hat{Q}_n \rho_{\text{tot}}^{-1}(0) \hat{P}_n \rho_{\text{tot}}(0) \hat{P}_n.$$
because the elements $\langle n(0)|\hat{\rho}_{\text{tot}}(0)|n(0)\rangle$ and $\langle m(T)|\hat{\rho}_{\text{tot}}(T)|m(T)\rangle$ are not $c$ numbers. Equation (35) reduces to (12) by eliminating the degrees of freedom of the reservoir. We will analyze the properties and the meanings of the corrections in equation (35) in section 4.

3.1. A case where the initial and the final states are product states

If the density matrix of the local system $\hat{n}(0)$ in (26) is measured at $t = 0$ and the result is an eigenstate $|n(0)\rangle$, we have $\hat{n}(0)\hat{P}_n = p_n \hat{P}_n$, where $p_n$ is the eigenvalue of $\hat{n}(0)$. Therefore, just as in the case of isolated systems, $g_n = p_n^{-1}p_n = 1$ and $\xi_\beta = 0$. If the final state is also a product state and the density matrix of the local system is measured at $t = T$ with the result of an eigenstate $|m(T)\rangle$, we have $\hat{n}(T)\hat{P}_m = p_m \hat{P}_m$, where $p_m$ is the eigenvalue of $\hat{n}(T)$; we have $\xi_\alpha = 0$ in this case. When both of these conditions are satisfied, the microscopic reversibility holds exactly:

$$p_F(|n(0)\rangle \rightarrow |m(T)\rangle) = p_R(\hat{\Theta}|m(T)\rangle \rightarrow \hat{\Theta}|n(0)\rangle).$$

(37)

This is another major result of the present paper. This means that no matter how strong the local system is connected to the reservoir during the period between the measurements, the microscopic reversibility holds as long as the above conditions are satisfied. Note that this is a sufficient condition; we are not yet sure what is the necessary condition to make the correction terms vanish.

3.2. A case where the local system is disconnected from the reservoir

Again, we consider the case where we measure the density matrix of the local system at $t = 0$ with the result of an eigenstate $|n(0)\rangle$. Now, let us consider the process where we gradually disconnect the local system from the reservoir and measure the energy of the local system at $t = T$ with the result of an energy eigenstate $|m(T)\rangle$. Here we do not assume the form of the density matrix at $t = T$.

If we split the time evolution at the time $\tau_{\text{iso}}$, at which we can regard that the local system is almost isolated from the reservoir, i.e.

$$\hat{U}(T) = \hat{U}(T - \tau_{\text{iso}}) \hat{U}(\tau_{\text{iso}}) = (\exp(-i\hat{H}_s(T - \tau_{\text{iso}})) \otimes \exp(-i\hat{H}_r(T - \tau_{\text{iso}})))\hat{U}(\tau_{\text{iso}}),$$

(38)

then we have

$$p_F(|n(0)\rangle \rightarrow |m(T)\rangle) = \text{Tr}_r(\langle n(0)|\hat{U}(\tau_{\text{iso}})|n(0)\rangle\hat{\rho}_{\text{tot}}(0)|n(0)\rangle\langle n(0)|\hat{U}^\dagger(\tau_{\text{iso}})|m(T)\rangle),$$

$$p_R(\Theta|m(T)\rangle \rightarrow \Theta|n(0)\rangle) = \text{Tr}_r(\langle n(0)|\hat{U}^\dagger(\tau_{\text{iso}})|m(T)\rangle|m(T)\rangle\hat{\rho}_{\text{tot}}(0)$$

$$\times \hat{U}^\dagger(\tau_{\text{iso}})|m(T)\rangle|m(T)\rangle\hat{U}(\tau_{\text{iso}})|n(0)\rangle),$$

(39)

which are independent of the state at $t = T$. Therefore, the transition probabilities and the correction term $\xi_\alpha$ become constant after the local system is completely disconnected.

Compared to the case of the isolated quantum systems, the behavior of the microscopic reversibility in open quantum systems is more nontrivial, depending on the protocol that we choose.

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4. Details of the corrections

We only consider the case of open quantum systems because the consequences for isolated systems follow by eliminating the degrees of freedom of the reservoir.

4.1. Correction factor $g_n$

Let us analyze the properties of the correction factor $g_n$. Introducing a unitary matrix $\hat{V}$ that transforms the density matrix of the local system $\hat{\rho}_s(0)$ in the present measurement basis to its diagonal form, i.e.

$$\hat{\rho}_s(0) = \hat{V} \hat{\rho}_D(0) \hat{V}^\dagger, \quad \hat{\rho}_D(0) = \text{diag}(p_1, p_2, \ldots, p_N),$$

we can write the general form of $g_n$ in (34) as

$$g_n = \sum_{i,j=1}^N \frac{p_i}{p_j} |v_{ni}|^2 |v_{nj}|^2,$$  

(41)

where $v_{ij}$ is the $(i,j)$ element of $\hat{V}$. We have $g_n = 1$ if we choose the state $|n(0)\rangle$ as an eigenstate of the density matrix of the local system. Since $\hat{\rho}_s(0)$ is a positive operator, $g_n$ is positive, which is also obvious from (41). The factor $g_n$ can be large if some states have a relatively small probability $p_j$ in the diagonalizing basis. Note, however, that $g_n$ is finite; to have $g_n = \infty$, it would require that $p_j = 0$ for the $j$th state, in which case the inverse of $\hat{\rho}_s(0)$ would not exist.

4.2. Correction terms $\xi_\alpha$ and $\xi_\beta$

The correction terms from the microscopic reversibility must be quantities related to the disturbance due to the measurement process. Here, we consider the quantities $\sigma_\alpha \equiv \xi_\alpha \hat{p}_R$ and $\sigma_\beta \equiv \xi_\beta \hat{p}_R$. We recast these correction terms into the forms

$$\sigma_\alpha = g_n \text{Tr} \, \hat{P}_n \hat{U}^\dagger \hat{P}_m \hat{\rho}_{tot}(T)(1 - \hat{P}_m) \hat{U}$$

$$= g_n \text{Tr} \, \hat{P}_n \hat{U}^\dagger \hat{P}_m \hat{\rho}_{tot}(T) \hat{U} - g_n \text{Tr} \, \hat{P}_n \hat{U}^\dagger \hat{P}_m \hat{\rho}_{tot}(T) \hat{P}_m \hat{U}$$

$$= g_n \text{Tr} \, \hat{P}_n \hat{U}^\dagger \hat{P}_m \hat{\rho}_{tot}(T) \hat{U} - g_n \hat{p}_R (\hat{\Theta} |m(T)\rangle \rightarrow \hat{\Theta} |n(0)\rangle),$$

(42)

and

$$\sigma_\beta = \text{Tr} \, \hat{P}_n \hat{U}^\dagger \hat{P}_m \hat{\rho}_{tot}(T) \hat{U} (1 - \hat{P}_n) \hat{\rho}_{tot}^{-1}(0) \hat{P}_n \hat{\rho}_{tot}(0)$$

$$= \text{Tr} \, \hat{P}_n \hat{U}^\dagger \hat{P}_m \hat{\rho}_{tot}(T) \hat{U} \hat{\rho}_{tot}^{-1}(0) \hat{P}_n \hat{\rho}_{tot}(0) - g_n \text{Tr} \, \hat{P}_n \hat{U}^\dagger \hat{P}_m \hat{\rho}_{tot}(T) \hat{U}$$

$$= \text{Tr} \, \hat{P}_n \hat{U}^\dagger \hat{P}_m \hat{\rho}_{tot}(0) - g_n \text{Tr} \, \hat{P}_n \hat{U}^\dagger \hat{P}_m \hat{\rho}_{tot}(T) \hat{U}$$

$$= p_F(|n(0)\rangle \rightarrow |m(T)\rangle) - g_n \text{Tr} \, \hat{P}_n \hat{U}^\dagger \hat{P}_m \hat{\rho}_{tot}(T) \hat{U}.$$

(43)
The Hamiltonian is the correction of the density matrix with respect to the degrees of freedom of the local system; therefore, the difference inside the parentheses in (44) comes from the off-diagonal elements of the eigenstate and \( \text{Tr} \hat{\rho}_{\text{tot}}(T) \hat{U} \).

The correction \( \sigma_{\alpha} \) is the quantity related to the effect that the measurement at the final moment destroys the quantum coherence. The correction \( \sigma_{\beta} \), on the other hand, depends on the factor \( g_n \) and is independent of the state at \( t = T \); therefore, the quantity \( \sigma_{\beta} \) is related to the fact that the measured state at the initial moment differs from the eigenstate of the density matrix of the local system. The factor \( 1 - g_n \) indicates the difference from the eigenstate and \( \text{Tr} \hat{P}_n \hat{\rho}_{\text{tot}}(0) \) is the probability of observing the state \( |n(0)\rangle \).

5. Example of an open quantum system: one-dimensional spin chain

In order to evaluate the value of the correction from the microscopic reversibility quantitatively, we will numerically treat an open quantum system with a finite-size reservoir.

5.1. Hamiltonian and protocol

Let us consider the total system which consists of \( N \) pieces of 1/2 spins. We regard the first \( N_s \) spins as the local system and the remaining \( N_r(=N - N_s) \) spins as the reservoir. The Hamiltonian is

\[
\hat{H}_{\text{tot}}(t) = \hat{H}_s(t) + \hat{H}_r(t) + \hat{H}_c \theta(t),
\]

\[
\hat{H}_s(t) = \sum_{i=1}^{N_s-1} J(\hat{S}_i^z \hat{S}_{i+1}^z + \theta(t)\hat{S}_i^x \hat{S}_{i+1}^x),
\]

\[
\hat{H}_r(t) = \sum_{i=N_s+1}^{N_s+N_r-1} J(\hat{S}_i^z \hat{S}_{i+1}^z + \theta(t)\hat{S}_i^x \hat{S}_{i+1}^x),
\]

\[
\hat{H}_c = J(\hat{S}_{N_s}^z \hat{S}_{N_s+1}^z + \hat{S}_{N_s}^x \hat{S}_{N_s+1}^x).
\]
Figure 2. The $T$ dependence of quantities for the spin chain with $N = 6–10$. The number of system spins is $N_s = 2$. We set $J = 0.1$, $\beta_s = 1$, $\beta_r = 0.1$ and consider the transition from $|n(0)\rangle = |\uparrow\downarrow\rangle$ to $|m(T)\rangle = (|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle)/\sqrt{2}$ as the forward process. The horizontal axis indicates the time $T$ at which we measure the local system. The plots show the $T$ dependence of (a) the forward transition probability $p_F(|n(0)\rangle \rightarrow |m(T)\rangle)$, (b) the reversed transition probability $p_R(\hat{\Theta}|m(T)\rangle \rightarrow \hat{\Theta}|n(0)\rangle)$, (c) the ratio of the forward and the reversed transition probabilities $p_F/p_R = 1 + \xi_\alpha$ and (d) the correction term $\sigma_\alpha = \xi_\alpha p_R$.

For $t < 0$, the total system consists of the two isolated Ising chains. We set them in the thermal equilibrium states at different inverse temperatures $\beta_s$ and $\beta_r$. At $t = 0$, we measure the energy of the local system; the measurement basis of the initial state is the eigenstate of the density matrix of the local system and thus $g_n = 1$, $\sigma_0 = \sigma_\beta = 0$ and $\sigma_T = \sigma_\alpha$. Then the local system is connected to the reservoir, so that for $t > 0$ the total system becomes an $XY$ model. Finally, we again measure the energy of the local system at $t = T$. The strength of $J$ is spatially uniform, and thus this is the case of strong coupling between the local system and the reservoir. This process satisfies the relation $\langle m(T)|\hat{\Theta}\hat{\rho}(T)\hat{\Theta}|m(T)\rangle = \langle m(T)|\hat{\rho}(T)|m(T)\rangle$ because the Hamiltonian is invariant under the flip of all spins. In order to calculate the time evolution, we diagonalize the Hamiltonian of the total system numerically with LAPACK.

5.2. Results

We set $N_s = 2$ and varied the number of reservoir spins $N_r$. Figure 2(a) shows the $T$ dependence of the forward transition probability $p_F(|n(0)\rangle \rightarrow |m(T)\rangle)$ that we obtain.

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the measurement results $|n(0)\rangle = |\uparrow\downarrow\rangle$ and $|m(T)\rangle = (|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle)/\sqrt{2}$, which are the energy eigenstates of the local system, while figure 2(b) shows the dependence of the corresponding reversed transition probability $p_R(\Theta|m(T)\rangle \rightarrow \Theta|n(0)\rangle)$. Figures 2(c) and (d) show the $T$ dependences of the correction terms $\xi_\alpha$ and $\sigma_\alpha$. We set the inverse temperatures $\beta_s = 1$ and $\beta_r = 0.1$ with the coupling strength $J = 0.1$. As long as the number of the reservoir spins $N_r$ is finite, the finite-size effect appears as the measurement time $T$ becomes large. We can, however, regard the local system as an open system up to $T \sim 150$ in the simulation for $N = 10$. It shows that the forward transition probability converges to a certain value which is presumably of a new equilibrium state for $t > 0$. The correction term $\xi_\alpha$ converges to a very small (but finite) value, i.e. $\xi_\alpha \ll 1$. It is rather surprising because, even though the local system approaches to an equilibrium state, the local system can be entangled with the reservoir strongly; the density matrix of the total system can be totally different from the product state and the measurement process could cause a large value of the correction term according to the discussion in section 3.

The correction seems to remain small generally in this model. We show in figure 3(a) the same quantity as in figure 2(c) in the case of $N = 8$, but by varying the value of the inverse temperatures of the local system $\beta_s$ and the reservoir $\beta_r$. For $T \sim 0$, the ratio is sensitive to the value of the temperature of the local system $\beta_s$. The ratio $p_F/p_R$ for each parameter, however, seems to converge to the same small value as the local system goes to the new equilibrium state. Figure 3(b) shows the same quantity as in figure 2(c) in the case of $N = 8$, but with the coupling strength $J$ varied. The time evolution of the system is fast for the system with a large value of $J$ and hence the period for which the system indicates the behavior of the open system is short. In the region where we can regard the evolution of the ratio $p_F/p_R$ of each parameter as the behavior of the open quantum system ($T \lesssim 90$ for $J = 0.08$, $T \lesssim 120$ for $J = 0.1$ and $T \lesssim 150$ for $J = 0.12$), the ratios also seem to converge to a common small value as the local system goes to the new equilibrium state. Finally, figures 4(a) and (b) show the cases of all possible combinations of the states $|n(0)\rangle$ and $|m(T)\rangle$. Although the sign is negative in the case of $|n(0)\rangle = |\uparrow\uparrow\rangle$, the absolute value of the ratio $p_F/p_R$ of each case seems to converge to a common small value. It is difficult to determine from the numerical calculations whether all these small

![Figure 3](image-url)
values of the ratio $p_F/p_R$ at the stationary states coincide with each other, but they are of the order of $10^{-4}$.

Further theoretical study is required to estimate the order of the correction term compared to the transition probabilities. Nevertheless, the present simulation suggests that we can expect that the microscopic reversibility in open quantum systems almost holds even when the local system cannot be regarded as macroscopic.

6. Conclusion

We derived the correction terms of the microscopic reversibility of isolated quantum systems (5) and (12) as well as of open quantum systems (35) by formal but exact treatment. Throughout the paper, we assumed the relation $\langle m(T) | \hat{\Theta} \hat{\rho}(T) \hat{\Theta} | m(T) \rangle = \langle m(T) | \hat{\rho}(T) | m(T) \rangle$ and the product initial state for open quantum systems.

We summarize the results of the present paper in table 1. For the microscopic reversibility in isolated quantum systems, we exemplified the case of a free-particle system and found that the correction term can be very large. For the microscopic reversibility in open quantum systems, we first considered two situations which seem to be physically important: the case where the correction terms vanish (section 3.1) and the case where we disconnect the local system from the reservoir in the middle of the time evolution (section 3.2). In section 4, we discussed the details of the corrections; we analyzed the bound of the factor $g_n$ and showed the meaning of the other correction terms explicitly by considering the quantities $\sum_m \sigma_t = \sum_m \xi_t p_R$ and $\sum_m \sigma_\beta = \sum_m \xi_\beta p_R$ in (44) and (45). Although we do not have an appropriate method of estimating the order of the correction terms theoretically, our numerical simulations of the one-dimensional spin chain suggested that, in the case of a thermal relaxation process, the correction term becomes very small compared to the transition probabilities; the microscopic reversibility almost holds even when the local system cannot be regarded as macroscopic.

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Table 1. The microscopic reversibility for each situation. The initial state is always assumed to be the product state for open systems.

| System | Initial measurement basis | Final state | Final measurement basis | Microscopic reversibility |
|--------|---------------------------|-------------|-------------------------|--------------------------|
| Isolated | Eigenstate of $\hat{\rho}(0)$ | Arbitrary | Eigenstate of $\hat{\rho}(T)$ | Exact |
| Isolated | Eigenstate of $\hat{\rho}(0)$ | Arbitrary | Arbitrary | Correction $\xi_\alpha$ (possibly huge) |
| Isolated | Arbitrary | Arbitrary | Arbitrary | Corrections $g_n, \xi_\alpha, \xi_\beta$ (possibly huge) |
| Open | Eigenstate of $\hat{\rho}_k(0)$ | Product state | Eigenstate of $\hat{\rho}_k(T)$ | Exact |
| Open | Arbitrary | Local system disconnected | Arbitrary | Constant corrections |
| Open | Eigenstate of $\hat{\rho}_k(0)$ | Arbitrary | Arbitrary | Correction $\xi_\alpha$ (seems small) |
| Open | Arbitrary | Arbitrary | Arbitrary | Corrections $g_n, \xi_\alpha, \xi_\beta$ |

We expect that further analyses of the microscopic reversibility will reveal more interesting properties of open quantum systems.

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