Microscopic reversibility of quantum open systems

Takaaki Monnai

Department of Applied Physics, Osaka City University, 3-3-138 Sugimoto, Sumiyoshi-ku, Osaka 558-8585, Japan
E-mail: monnai@a-phys.eng.osaka-cu.ac.jp

Received 20 January 2012, in final form 10 February 2012
Published 6 March 2012
Online at stacks.iop.org/JPhysA/45/125001

Abstract

The transition probability of an isolated system for a time-dependent unitary evolution is invariant under the reversal of protocols. In this paper, we generalize the expression of microscopic reversibility to externally perturbed large quantum open systems, which provides a model-independent equality between time forward and reversed joint transition probabilities. A time-dependent external perturbation acts on the subsystem during a transient duration, and subsequently the perturbation is switched off so that the total system would thermalize. We concern ourselves with the net transition probability for the subsystem from the initial to final states after a time evolution during which the energy is irreversibly exchanged between the subsystem and reservoir. The time-reversed probability is given by the reversal of the forcing protocol and the initial ensemble. Microscopic reversibility equates the time forward and reversed probabilities, and therefore appears as a thermodynamic symmetry for open quantum systems.

PACS numbers: 05.30−d, 05.70−Ln

(Some figures may appear in colour only in the online journal)

Microscopic reversibility of the unitary evolution plays a key role in the foundation of nonequilibrium statistical mechanics. Indeed, the time-reversal invariance of the equation of motions amounts to universal symmetry of fluctuation theorems and related equalities [1–19] for the fluctuation of entropy production and particle current for mesoscopic systems, and thus plays fundamental role in the nonequilibrium statistical mechanics. The symmetries connect the probabilities of positive and negative entropy production [9, 20], which are calculated from the time forward and reversed transition probabilities for quantum systems [4, 5, 13, 15–17].

In the classical Markovian stochastic dynamics, the conditional probability functional of the trajectories satisfies a symmetry expressed by the probability functionals and heat. This relation is also called microscopic reversibility [9] and generalized to the quantum open systems by concerning the heat calculated from a set of transitions of the reservoir states [10, 11].
On the contrary, we are interested in the joint transition probabilities between the system states instead of the statistics for continuously monitored heat and give an expression of microscopic reversibility based on the macroscopic properties of quantum open systems. As a complementary work of the preliminary version of this paper, reference [23] rigorously analyzes the validity of the microscopic reversibility and numerically shows that it seems to hold provided that the thermalization occurs after a quench. Here, we reveal the mechanism how the thermalization hypothesis amounts to the expression of the microscopic reversibility.

The manipulation and thermalization of quantum open systems are of great interest for the tunable cold atoms and the tunneling in molecular magnets. As a concrete example of the transition of the system states, we remark that the induced absorption and emission between two levels by an external electric field are equally probable within the realm of Fermi’s golden rule, provided that the initial and final Fock states are exchanged. The absorption process can be seen as the time reversal of the corresponding emission process.

In this paper, we show that a model-independent time-reversal symmetry similar to that of the induced absorption holds for generic macroscopic time-dependent open systems where the system couples to the reservoir. Since the expression appears as a generic equation for the forward and reversed forcing protocols, we call it microscopic reversibility.

The paper is organized as follows. First, we describe our model and forcing protocol. An expression of microscopic reversibility for open systems is derived in equation (14). Then, the microscopic reversibility is numerically verified.

1. Model

Let us consider a finite system interacting with a macroscopically large reservoir at an inverse temperature $\beta$. The system is externally controlled by a time-dependent parameter $\lambda(t)$, which is for example a spring constant for the case of a harmonic oscillator.

The total Hamiltonian is

$$H(t) = H_s(\lambda(t)) + H_r + H_{sr},$$

(1)

where $H_s(\lambda(t))$, $H_r$ and $H_{sr}$ are the Hamiltonians of the system, reservoir and interaction between them, respectively.

Let us prepare the initial state as

$$\rho(0) = \rho_s(\lambda(0)) \otimes \rho_r,$$

$$\rho_s(\lambda(0)) = \frac{e^{-\beta H_s(\lambda(0))}}{Z(\lambda(0))},$$

(2)

which is the product of the canonical ensembles of the system $\rho_s(\lambda(0))$ and of the reservoir $\rho_r$ at the same inverse temperature $\beta$. The partition function of the system is from the normalization

$$Z(\lambda(0)) = \text{Tr}_s e^{-\beta H_s(\lambda(0))}.$$  

(3)

Throughout this paper, we assume that the interaction energy $H_{sr}$ is regarded as small compared to the energy of the subsystem $H_s$ and the reservoir $H_r$. This assumption is reasonable for macroscopic systems, since $H_s$ and $H_r$ are the bulk energies, while $H_{sr}$ would be proportional to the surface area, which is relatively small compared to the volume. Note that the assumption is different from the weak coupling limit. Namely the weak coupling assumes that interaction is negligible, and the perturbative analysis is available. On the other hand, in our case the interaction is not necessarily vanishing, and we require only that the ratio between the interaction energy and bulk energy is negligible.
2. Twice measurements scheme

Twice measurements scheme consists of the initial and final observations which are described in (i) and (ii).

(i) At \( t = 0 \), we measure the energy operator of the system \( H_s(\lambda(0)) \) and gain an eigenenergy \( E_n(0) \). The system state becomes the corresponding eigenstate \( |n(0)\rangle \).

\[
H_s(\lambda(0))|n(0)\rangle = E_n(0)|n(0)\rangle. \tag{4}
\]

Subsequently, the total density matrix unitarily evolves until \( t = T \) as

\[
\rho(T) = U(|n(0)\rangle e^{-\beta E_n(0)} \frac{1}{Z(\lambda(0))} Z(\lambda(0)) \otimes \rho_r) U^+. \tag{5}
\]

Note that the density matrix takes into account the initial statistical weight \( e^{-\beta E_n(0)} \frac{1}{Z(\lambda(0))} Z(\lambda(0)) \) as a conditional probability. Here, \( U = T[e^{-\frac{i}{\hbar} \int_0^T d\lambda H_s(\lambda)}] \) is the unitary time evolution operator acting on the total state. For the time evolution, we assume that the external forcing is switched off well in advance at \( t = T \) and the total density matrix would relax to an equilibrium state at \( t = T \).

2.1. Thermalization hypothesis

\[
U \rho(0) U^+ \cong \rho_s(\lambda(T)) \otimes \rho_r, \quad \rho_s(\lambda(T)) = e^{-\beta H_s(\lambda(T))} \frac{1}{Z(\lambda(T))}. \tag{6}
\]

Here \( H_s(\lambda(T)) \) is the energy operator at \( t = T \) and \( Z(\lambda(T)) \) is the partition function.

We shall explain this quasi-equality. Quasi-equality (6) is derived from two major steps (a) and (b), and justified by a numerical verification (figure 1) of its consequence (equation (14)).
(a) After a thermalization until \( t = T \), we regard \( U_\rho(0)U^+ \) as indistinguishable from a reduced density matrix \( \text{Tr}_r |\psi\rangle \langle \psi| \) of a randomly sampled pure state \( |\psi\rangle \) extracted from the Hilbert space \( \mathcal{H}_{[E,E+\Delta E]} \) at an energy scale \( E \). Then, the equation at the level of matrix elements \([21, 22]\)

\[
\text{Tr}_r U \rho(0)U^+ \cong \rho_s(\lambda(T))
\]

holds because the randomly sampled state from an extremely high-dimensional Hilbert space almost always yields the reduced density matrix which is equal to the thermal state, and gives an evaluation of the time-evolved reduced density matrix of the system. The state \( \rho_s(\lambda(T)) \) is a canonical state at the inverse temperature \( \beta \) which is equal to that of the reservoir, because the reservoir is sufficiently large and its density matrix is almost invariant.

(b) Then, both the reduced and reservoir density matrices are close to equilibrium at the same temperature, and the total density matrix would be proportional to \( e^{-\beta(H_s(\lambda(T)) + H_r)} \).

Finally, from the assumption of relative smallness of the interaction energy, the total density matrix is well described by \( \rho_s(\lambda(T)) \otimes \rho_r \).

2.2. Remarks on the thermalization

Note that the above explanation is hypothetical, but provides a reason why its consequent microscopic reversibility holds when \( \rho(0) \) is a product state \([23]\). Researchers familiar with entanglement would also anticipate whether equation (6) is available for the calculation of all the observables. Actually, it would not capture macroscopic entanglements between the system and the reservoir; however, this is not a real problem, since in equation (14) it is acted by \( \rho_s(\lambda(T))^{-\frac{1}{2}} \times \rho_r^{-\frac{1}{2}} \) which clearly distinguishes the system and reservoir degrees of freedoms as a product.

(ii) At \( t = T \), we measure the energy \( H_s(\lambda(T)) \) and obtain some eigenenergy \( E_m(T) \) with the corresponding eigenvector \( |m(T)\rangle \). Regarding the reservoir, we do not perform any measurements. The net transition probability that the initial and final system states are \( |n(0)\rangle \) and \( |m(T)\rangle \) is then

\[
P_T(|n(0)\rangle \rightarrow |m(T)\rangle) = \text{Tr}_r\{ |m(T)\rangle U |n(0)\rangle \frac{e^{-\beta E_m(0)}}{Z(\lambda(0))} \rho_r(0[U^+ |m(T)\rangle] \}.
\]

Note that equation (8) defines a joint transition probability. Equation (8) is composed of the operator

\[
A_{nm} = \frac{1}{\sqrt{Z(\lambda(0))}} \frac{e^{-\beta E_n(0)}}{Z(\lambda(0))} |m(T)\rangle U |n(0)\rangle
\]

describing the transition of the system state, and satisfies

\[
\sum_{n,m} A^+_{nm} A_{nm} = \sum_n \frac{1}{Z(\lambda(0))} e^{-\beta H_s(\lambda(0))} U^+ \sum_m |m(T)\rangle \langle m(T) | U |n(0)\rangle = 1.
\]

Note that the matrix elements such as \( \langle m(T) | U |n(0)\rangle \) contain the reservoir variables, because \( U \) contains both system and reservoir degrees of freedom. The second equality follows from the completeness \( \sum_m |m(T)\rangle \langle m(T) | = 1 \), and the unitarity \( U^+ U = 1 \).

Similarly the probability of the time-reversed dynamics is also calculated. Firstly, let us define the reversed dynamics by reversing the time dependence of the system Hamiltonian in equation (2) as \( H_s(\lambda(T - t)) \), i.e. the reversal at time \( T \). Also, we start with the initial
state $\Theta e^{-\beta H_s(T)} \otimes \rho_s \Theta^{-1}$, where $\Theta$ is the anti-unitary time-reversal operator of the total system. The partition function is defined as

$$Z(\lambda(T)) \equiv \text{Tr}_s e^{-\beta H_s(\lambda(T))}. \quad (11)$$

(i) We measure the energy $\Theta H_s(\lambda(T)) \Theta^{-1}$ at $t = 0$ and gain the eigenenergy $E_m(T)$, and the system state becomes $\Theta |m(T)\rangle$. $\Theta |m(T)\rangle$ is proportional to $|m(T)\rangle$ when the energy $E_m(T)$ does not degenerate.

(ii) At the final time $t = T$, we again measure the energy $\Theta H_s(\lambda(0)) \Theta^{-1}$ and obtain the eigenenergy $E_n(0)$. The system state is $\Theta |n(0)\rangle$.

Then, the probability that the initial and final states are $\Theta |m(T)\rangle$ and $\Theta |n(0)\rangle$ for the reversed dynamics is

$$P_k(\Theta |m(T)\rangle \rightarrow \Theta |n(0)\rangle) = \text{Tr}_r \{ |n(0)\rangle \langle T U^+ \Theta |m(T)\rangle e^{-\beta E_n(T)} Z(\lambda(T))^{1/2} \rho_s |m(T)\rangle \langle T U \Theta |n(0)\rangle \}. \quad (12)$$

Here $\langle n(0)\rangle \langle T U^+ \Theta |m(T)\rangle = \langle m(T)| U |n(0)\rangle$ is the inner product of $\Theta |n(0)\rangle$ and $U^+ \Theta |m(T)\rangle$.

3. Microscopic reversibility

Now let us show a microscopic reversibility expressed by net probabilities of the forward and reversed transitions:

$$P_F(|m(0)\rangle \rightarrow |n(T)\rangle) \equiv P_F(\Theta |n(T)\rangle \rightarrow |m(0)\rangle). \quad (13)$$

Here the difference between the forward and reversed probabilities would go to zero in the macroscopic limit. A condition for thermalization, to regard the time-evolved state as a reduced density matrix of a randomly sampled state, would be available in this case. Note that $P_F(|m(0)\rangle \rightarrow |n(T)\rangle)$ is a net transition probability, which amounts to an absence of an exponential activation factor in equation (13) that appears in the fluctuation theorem. The microscopic reversibility (13) provides a generic symmetry, and is useful to verify the thermalization hypothesis.

In order to derive equation (13), we apply the methodology developed in [10, 11] and thermalization property (6). We rewrite the forward probability as

$$P_F(|m(0)\rangle \rightarrow |n(T)\rangle) = \text{Tr}_r \{ |n(T)\rangle U |m(0)\rangle \langle m(0)| \rho_s(\lambda(0)) \rho_r |m(0)\rangle \langle m(0)| U^+ |n(T)\rangle \}
$$

$$= \text{Tr}_r \rho_r^{-1} |m(0)\rangle \langle Z(\lambda(0))^{1/2} e^{-\beta H_s(\lambda(0))} U^+ |n(T)\rangle \}
$$

$$= \text{Tr}_r \rho_r^{-1} |m(0)\rangle \langle Z(\lambda(0))^{1/2} e^{-\beta H_s(\lambda(0))} |m(0)\rangle \}
$$

$$= \text{Tr}_r |n(T)\rangle U^+ \{ |U \rho_s(\lambda(0)) \rho_r(\lambda(T))^{-1} \rho_r^{-1} |U \rho_s(\lambda(0)) \rho_r(\lambda(T))^{-1} \rho_r^{-1} U^+ |m(0)\rangle \}
$$

$$= \text{Tr}_r |n(T)\rangle U^+ \{ |U \rho_s(\lambda(0)) \rho_r(\lambda(T))^{-1} \rho_r^{-1} U^+ |m(0)\rangle \}
$$

$$= \text{Tr}_r |n(T)\rangle U^+ \{ \frac{1}{Z(\lambda(T))} e^{-\beta E_s(T)} |n(T)\rangle \}
$$

$$= \frac{1}{Z(\lambda(T))} e^{-\beta E_s(T)} \text{Tr}_r |m(0)\rangle U^+ |n(T)\rangle \rho_r |n(T)\rangle |m(0)\rangle
$$

$$= P_k(\Theta |n(T)\rangle \rightarrow \Theta |m(0)\rangle). \quad (14)$$
The second equality derived from the cyclic property of the trace where we decomposed \( \rho_r \) into \( \rho_r^{1/2} \rho_r^{-1/2} \) and \( \rho_r^{-1/2} \rho_r^{1/2} = 1 \) is inserted in the middle. Also note that \( \rho_r(\lambda(0)) = \rho_r(\lambda(0))^{1/2} \rho_r(\lambda(0))^{1/2} \) becomes the real number \( \frac{1}{\sqrt{\text{tr}(\rho_r)}} \) e\(^{-\frac{1}{2}\beta}\text{E}(0)\) when acting on the eigenstates \( |m(0)\rangle \) and \( \langle m(0)| \). In the third equality, \( U^*U = 1 \) is inserted twice just after \( |m(0)\rangle \) and before \( \langle m(0)| \). \( \rho_r^{1/2} \) commutes with system variables such as \( |m(0)\rangle \) and \( \rho_r(\lambda(0))^{1/2} \).

Also, with the use of the relaxation property of the density matrix (6) which comes from equation (7) and the smallness of the interaction energy \( \mathcal{H}_r \) with respect to the bulk energy, the contents of the curly brackets \( U \rho_r(\lambda(0))^{1/2} \rho_r^{1/2} U^* \equiv \rho_r(\lambda(T))^{1/2} \rho_r^{1/2} \) are just the inverse of the remaining quantities in the brackets \( \rho_r(\lambda(T))^{-1} \rho_r^{-1} \).

### 4. Numerical demonstration of microscopic reversibility

In this section, we numerically show the microscopic reversibility (14). See also the detailed numerical verification in [23] for various parameters and measurement basis. We consider \( N = 8 \) site spin chain in the spatially inhomogeneous time-dependent magnetic field. Note that thermalization property has been observed in relatively small system sizes [24, 25], and this is true also for our case. Let us explain why such a short chain can exhibit the relaxation phenomena. The deviation of a state from equilibrium is typically bounded by the inverse of the dimension of the Hilbert space, which exponentially depends on the system size.

The Hamiltonian is given as

\[
\mathcal{H}(t) = \mathcal{H}_s(t) + \mathcal{H}_r(t) + \mathcal{H}_m,
\]

\[
\mathcal{H}_s(t) = -J_s \sum_{j=1}^{N_s-1} \sigma_j^x \sigma_{j+1}^x + \alpha_s \sum_{j=1}^{N_s-1} \sigma_j^z + \mu(t) \sum_{j=1}^{N_s-1} \sigma_j^z
\]

\[
\mathcal{H}_r = -J_r \sum_{j=J_s+1}^{N} \sigma_j^x \sigma_{j+1}^x + \alpha_r \sum_{j=J_s+1}^{N} \sigma_j^z + \gamma_r \sum_{j=J_s+1}^{N} \sigma_j^z
\]

\[
\mathcal{H}_m = -J_m \sigma_{N_s}^x \sigma_{N_s+1}^x + \alpha_m \sigma_{N_s}^z + \gamma_m \sigma_{N_s}^z,
\]

where \( \sigma_j^i \) is the \( i \) component of the Pauli matrix on the \( j \)th site. The sites \( j = 1, 2 (N_s = 2) \) and \( 3 < j \leq N \) are regarded as the subsystem and reservoir. The external magnetic field \( h(t) = \frac{B}{2} - \frac{B}{2} \tan(\mu(t - \tau)) \) satisfies \( h(0) \equiv B \) and is switched off after \( t = \tau \). The initial state is prepared as

\[
\rho(0) = \rho_r(0) \rho_r ;
\]

\[
\rho_r(0) = \frac{1}{Z_r(0)} e^{-\beta \mathcal{H}_r(0)},
\]

\[
\rho_r = \frac{1}{Z_r} e^{-\beta \mathcal{H}_r}
\]

We calculated the forward and reversed transition probabilities in figure 1. The parameters are chosen as follows. The exchange interactions at each site are \( J_s = J_r = J_m = 1 \), the \( x \) component of the magnetic field is expressed by the parameters \( \alpha_s = \alpha_r = 1 \), \( \alpha_m = 0.2 \), and similarly the \( z \) component of the magnetic field is given by \( h(t) \) with \( B = 3 \), \( \mu = 5 \), \( \gamma_r = 1 \) and \( \gamma_m = 0.2 \). The parameters \( \alpha_m \) and \( \gamma_m \) are chosen relatively small so that the interaction energy is small compared with the bulk energy. The inverse temperature is \( \beta = 0.01 \) and the switching time is \( \tau = 5 \).

The unitary time evolution \( U = T \{ e^{-i \int_0^T \mathcal{H}(t) dt} \} \) is discretized as \( e^{-i \Delta t \mathcal{H}(N \Delta t)} e^{-i \Delta t \mathcal{H}((N-1) \Delta t)} \cdots e^{-i \Delta t \mathcal{H}(\Delta t)} e^{-i \Delta t \mathcal{H}(0)} \) with the time step \( \Delta t = 0.05 \) which is much shorter than the time scale of the external perturbation. Initially, we measure the eigenstate of
$H_s(0)$ corresponding to the largest eigenvalue. The measurement basis at $t = T$ is chosen as the eigenstate of $H_s(T)$ which corresponds to the second largest eigenvalue. Note that there are no crossing of time-dependent energy levels of the subsystem, and equation (13) also holds for the transitions to other three eigenstates. It is remarkable that the time dependence of the forward and reversed transition probabilities is similar as a function of time even after the quench at $t \approx \tau$.

5. Summary

We have derived a model-independent expression of microscopic reversibility for macroscopic quantum open systems. The microscopic reversibility is trivial for the transition probability of unitary time evolution for the total system. Similar reversibility is well known for the transition probabilities of the induced absorption and emission under the influence of an electric field. The microscopic reversibility (13) is regarded as a generalization to the case of generic time-dependent perturbation. Therefore, it is a symmetry that holds in generic macroscopic quantum open systems. The microscopic reversibility is numerically verified for a spin chain in the presence of a time-dependent perturbation.

We shall refer to the related works here. Stimulated by the preliminary version of this paper, reference [23] provides a microscopic analysis of the validity of the microscopic reversibility. It confirms that microscopic reversibility holds provided that the initial product state is suddenly quenched and isolated to achieve thermalization. Our derivation (14) clarifies the mechanism where the thermalization process actually amounts to the microscopic reversibility.

In the context of the quantum generalization of the reversibility for the classical conditional probability functional, reference [10] derives another symmetry for the quantum trajectories. The main difference from [10] is the quantity which we measure, number of measurements and the definition of the reversed process. Here, we pursue and measure the system states. This is a useful property of the present scheme, since the system variables are expected to be much easier to measure with sufficient accuracy compared to those of the spatially extended large reservoir. The number of measurements is kept minimum here, but in [10] the reservoir state is frequently measured to define the quantum trajectory. In [9], the definition of the reversed process is based on the reversed ordering of the Kraus operators, while it is here defined by a reversed unitary time evolution.

Acknowledgments

TM is grateful to Professor S Tasaki for his encouragement and Professor A Sugita for fruitful discussions. This work is supported by the JSPS research program under the grant 22·7744.

References

[1] Jarzynski C 2000 J. Stat. Phys. 98 77–102
[2] Evans D J, Cohen E G D and Morriss G P 1993 Phys. Rev. Lett. 71 2401
[3] Gallavotti G and Cohen E G D 1995 J. Stat. Phys. 80 931
[4] Kurchan J 2000 arXiv:cond-mat:0007360
[5] Tasaki S and Matsui T 2003 Quantum Prob. White Noise Anal. 17 100–19
[6] Callens I, De Roeck W, Jacobs T, Maes C and Netočný K 2004 Physica D 187 383–91
[7] Gelin M F and Kosov D S 2008 Phys. Rev. E 78 011116
[8] Jarzynski C 1997 Phys. Rev. Lett. 78 2690
   Jarzynski C 1997 Phys. Rev. E 56 5018
[9] Crooks G E 1999 \textit{Phys. Rev. E} \textbf{60} 2721
Crooks G E 2000 \textit{Phys. Rev. E} \textbf{61} 2361
[10] Crooks G E 2008 \textit{Phys. Rev. A} \textbf{77} 034101
[11] Crooks G E 2008 \textit{J. Stat. Mech.: Theor. Exp.} P10023
[12] Campisi M, Talkner P and Hanggi P 2009 \textit{Phys. Rev. Lett.} \textbf{102} 210401
[13] Andrieux D and Gaspard P 2008 \textit{Phys. Rev. Lett.} \textbf{100} 230404
[14] Andrieux D, Gaspard P, Monnai T and Tasaki S 2009 \textit{New J. Phys.} \textbf{11} 043014
[15] Monnai T 2005 \textit{Phys. Rev. E} \textbf{72} 027102
[16] Monnai Takaaki 2010 \textit{Phys. Rev. E} \textbf{81} 011129
[17] Saito K and Utsumi Y 2008 \textit{Phys. Rev. B} \textbf{78} 115429
[18] Esposito M, Harbola U and Mukamel S 2007 \textit{Phys. Rev. E} \textbf{76} 031132
[19] Esposito M, Harbola U and Mukamel S 2009 \textit{Rev. Mod. Phys.} \textbf{81} 1665
[20] Esposito M, Lindenberg K and Van den Broeck C 2010 \textit{New J. Phys.} \textbf{12} 013013
[21] Goldstein S, Lebowitz J L, Tumulka R and Zanghi N 2006 \textit{Phys. Rev. Lett.} \textbf{96} 050403
[22] Popescu S, Short A J and Winter A 2006 \textit{Nature Phys.} \textbf{2} 754–8
[23] Kawamoto T 2011 \textit{J. Stat. Mech.: Theor. Exp.} P10109
[24] Saito K, Takesue S and Miyashita S 1996 \textit{J. Phys. Soc. Japan.} \textbf{65} 1243–9
[25] Jensen R V and Shankar R 1985 \textit{Phys. Rev. Lett.} \textbf{54} 1879