On the Lindblad equation for open quantum systems: Rényi entropy rate and weak invariants

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Abstract. A brief review of two recent topics on the Lindblad equation is presented. One is concerned with time evolution of the quantum Rényi entropy under the equation. The lower bound of the entropy rate is derived in a compact form. The other is about the concept of weak invariants, which generalize the Lewis-Riesenfeld invariant and are defined in such a way that they are not constant but their expectation values remain invariant in time. The Lindbladian operator describing the time-dependent damped quantum oscillator is identified, and the corresponding weak invariant is explicitly constructed as an example.

1. Introduction
There is growing new interest in quantum theory of open systems. This stream has originated from areas of contemporary importance such as nanoscience and quantum information. There, deeper understanding of quantum entanglement, decoherence and thermalization is desired. Here, we discuss a couple of recent topics in quantum theory of open systems: time evolution of the quantum Rényi entropy and the concept of weak invariants. We develop discussions about them based on the Lindblad equation \cite{1,2}, which is the most general linear Markovian quantum master equation that preserves positive semidefiniteness of a density operator and generates a dynamical semigroup.

The present article is organized as follows. In Section 2, an elementary explanation is presented about the Lindblad equation. In Section 3, the general lower bound of the Rényi entropy rate under the Lindblad equation is discussed. In Section 4, the concept of weak invariants is formulated. As an example, the weak invariant of the time-dependent damped quantum oscillator is explicitly constructed. Section 5 is devoted to concluding remarks.

Throughout this article, $\hbar$ is set equal to unity for the sake of simplicity.

2. Lindblad equation
Consider an objective system $A$ and the environment $B$ that jointly form an isolated system. Assume that at certain time $t$ the total system is in an unentangled pure state, $|\Psi(t)\rangle_{AB} = |\psi(t)\rangle_A |\phi(t)\rangle_B$. Time evolution of this state may be given by a transformation: $|\Psi(t)\rangle_{AB} \rightarrow |\Psi(t')\rangle_{AB} = U_{AB}(t', t) |\Psi(t)\rangle_{AB}$, where $U_{AB}(t', t)$ is a unitary time-evolution operator. $U_{AB}$ is termed a local unitary operator if it has the form, $U_{AB} = U_A \otimes U_B$, where $U_A(U_B)$ is a unitary
operator in the space of the system $A$ ($B$). Clearly, a local unitary time-evolution operator does not induce entanglement between $A$ and $B$, and accordingly the marginal density operator of $A$, $\rho_A(t') = \text{tr}_B[|\Psi(t')\rangle_A\langle \Psi(t')|]$, remains pure, where the symbol $\text{tr}_B$ denotes the partial trace over $B$. Therefore, what is of interest is the case when $U_{AB}$ is nonlocal. Nonlocality can be realized if there exists an interaction between $A$ and $B$. Then, the total Hamiltonian, which generates time evolution of $|\Psi(t)\rangle_{AB}$, reads $H_{\text{tot}} = H_A + H_B + H_{AB}$, where $H_A(H_B)$ and $H_{AB}$ are the Hamiltonians of $A$ ($B$) and the interaction, respectively. The marginal density operator of $A$ is written as follows:

$$\rho_A(t') = \sum_i V_i(t', t)\rho_A(t)V_i^\dagger(t', t),$$

(1)

where $\rho_A(t) = |\psi(t)\rangle_A\langle \psi(t)|$ is the pure-state density operator of $A$ at $t$ and $V_i$ is the operator given by

$$V_i(t', t) = B\langle v_i|U_{AB}(t', t)|\phi(t)\rangle_B$$

(2)

with $\{|v_i\rangle_B\}_i$ being a certain complete orthonormal system in the space of $B$. Since $U_{AB}$ is unitary, $\text{tr}_A\rho_A(t') = \text{tr}_A\rho_A(t) = 1$, which leads to the trace-preserving condition

$$\sum_i V_i^\dagger V_i = I_A,$$

(3)

where $I_A$ is the identity operator in the space of $A$.

Equation (1) is referred to as the Kraus representation [3] in the literature and gives an example of completely positive maps. The set $\{V_i^\dagger V_i\}_i$ satisfying Eq. (3) is called a positive operator-valued measure commonly abbreviated as POVM.

Let us consider infinitesimal time evolution from $t$ to $t' = t + \Delta t$ [4]. We pick up one from $V_i$’s, say $V_0$, and write it as

$$V_0(t + \Delta t, t) = I_A - i\Delta tH_A - \sum_{i\neq 0}^\Delta \sum_i |g_i|^2 L_i^\dagger L_i + O((\Delta t)^2),$$

(4)

and the rest as

$$V_i(t + \Delta t, t) = (\Delta t)^{\frac{1}{2}}g_iL_i + O(\Delta t) \quad (i \neq 0),$$

(5)

where $g_i$’s are constant and the operators $L_i$’s may depend on $t$. From these, we ascertain that Eq. (3) holds up to the first order of $\Delta t$.

Substituting Eqs. (4) and (5) into Eq. (1) with $t' = t + \Delta t$, we have

$$\rho_A(t + \Delta t) = \rho_A(t) - i\Delta t[H_A, \rho_A(t)] - \frac{\Delta t}{2}\sum_{i\neq 0}^\Delta |g_i|^2 (L_i^\dagger L_i\rho_A(t) + \rho_A(t)L_i^\dagger L_i - 2L_i\rho_A(t)L_i^\dagger) + O((\Delta t)^{3/2}),$$

(6)

from which we obtain in the limit $\Delta t \to 0$ the Lindblad equation [1,2]:

$$i\frac{\partial \rho}{\partial t} = [H, \rho] - \sum_k c_k(L_k^\dagger L_k \rho + \rho L_k^\dagger L_k - 2L_k \rho L_k^\dagger),$$

(7)

which is local in time, i.e., Markovian. $k$ runs over the set of $i$ except $i = 0$ and $c_k = |g_k|^2$. Here and hereafter, the subscript “$A$” is omitted.

Nonnegativity of $c_k$’s is crucial for the density operator to remain positive semidefinite. To see this point, let us perform instantaneous diagonalization:

$$\rho(t) = \sum_\lambda p_\lambda(t)|u_\lambda(t)\rangle\langle u_\lambda(t)|,$$

(8)
Here, \(0 \leq p_\lambda(t) \leq 1\) and \(\sum_\lambda p_\lambda(t) = 1\). \{ |u_\lambda(t)\rangle \}_\lambda\) is a complete orthonormal system, which consists of the eigenstates of \(\rho(t)\) itself with the eigenvalues \(p_\lambda(t)\)'s. Suppose \(p_1(t) = 0\). Then, the \((1,1)\)-element of \(\partial \rho(t)/\partial t\) is given by \(\langle u_1(t)|\partial \rho(t)/\partial t|u_1(t)\rangle = dp_1(t)/dt\), provided that the condition \(\langle u_\lambda(t)|u_{\lambda'}(t)\rangle = \delta_{\lambda\lambda'}\) has been used. Therefore, from Eq. (7), we have \(dp_1/dt = \sum_k c_k \sum_{\lambda \neq 1} p_\lambda(t) |\langle u_1(t)|L_k|u_\lambda(t)\rangle|^2 \geq 0\), which guarantees that \(p_1(t)\) never becomes negative.

3. Rényi entropy rate under Lindblad equation

Characterizing entanglement is of crucial importance in diverse areas in contemporary physics from quantum theory of spacetime [6] to quantum information [7]. In recent years, the quantum Rényi entropy has repeatedly been examined as a useful measure of entanglement. Considering the Rényi entropy rate may shed light on entanglement dynamics.

The quantum Rényi entropy of a density operator \(\rho\) is defined by

\[
S_\alpha = \frac{1}{1-\alpha} \ln(\text{tr} \rho^\alpha),
\]

where \(\alpha\) is a positive index. This quantity converges to the von Neumann entropy \(S = -\text{tr}(\rho \ln \rho)\) in the limit \(\alpha \to 1\). \(\alpha\) as a parameter plays a convenient role in probing entanglement (see [8-10], for example). In the diagonal form of the density operator in Eq. (8), Eq. (9) is rewritten as follows:

\[
S_\alpha = \frac{1}{1-\alpha} \ln \left( \sum_\lambda p_\lambda^\alpha \right),
\]

which is formally equivalent to the original expression of the classical Rényi entropy [11].

A couple of comments are made on the Rényi entropy. Firstly, not only the Rényi entropy but also any other generalized entropy cannot be the thermodynamic entropy. Maximum entropy methods with generalized entropies violate the Shore-Johnson axioms [12-14], and therefore artificial biases are introduced into such inference schemes [15,16]. Secondly, the Rényi entropy is as a functional not uniformly continuous in the limit of a large number of microscopically accessible states. This issue is concerned with the so-called Lesche stability [17] (see also [18]). It implies that the values of the Rényi entropy for two distributions slightly different from each other can largely be different.

Let us proceed to a discussion about time evolution of the Rényi entropy under the Lindblad equation. Taking the time derivative of the Rényi entropy and using Eq. (7), we have

\[
\frac{dS_\alpha}{dt} = \frac{1}{\text{tr} \rho^\alpha} \sum_k c_k G_k,
\]

where

\[
G_k = \frac{\alpha}{1-\alpha} \text{tr}(\rho^{\alpha-1} L_k \rho L_k^\dagger - \rho^\alpha L_k^\dagger L_k).
\]

Substituting the instantaneously diagonalized form of the density operator in Eq. (8) into Eq. (12), we have

\[
G_k = \frac{\alpha}{1-\alpha} \left( \sum_{\lambda \mu} p_\lambda^{\alpha-1} p_{\mu} |\langle u_\lambda|L_k|u_\mu\rangle|^2 - \sum_\lambda p_\lambda^\alpha |\langle u_\lambda|L_k^\dagger L_k|u_\lambda\rangle|^2 \right).
\]

Here and hereafter, the density operator is assumed to be positive definite. To further evaluate this quantity, we consider a function \(f(x) = x^\alpha\) defined for positive \(x\), which is concave (convex) if \(0 < \alpha < 1\) \((\alpha > 1)\). That is,

\[
[r p_\lambda + (1-r)p_\mu]^\alpha > r p_\lambda^\alpha + (1-r)p_\mu^\alpha \quad (0 < \alpha < 1),
\]

where 0 ≤ \(r\) ≤ 1.
\[ [rp_\lambda + (1 - r)p_\mu]^\alpha < rp_\lambda^\alpha + (1 - r)p_\mu^\alpha \quad (\alpha > 1), \]  
where \( 0 < r < 1 \). In addition, the following inequalities hold for \( y > 0 \): \( y^\alpha - 1 \leq \alpha(y - 1) \) \( (0 < \alpha < 1) \), \( y^\alpha - 1 \geq \alpha(y - 1) \) \( (\alpha > 1) \), with the equalities for \( y = 1 \). Combining these with Eqs. (14) and (15), we have the following relations:

\[ \alpha p_\lambda^{\alpha - 1} p_\mu > (\alpha - 1)p_\lambda^\alpha + p_\mu^\alpha \quad (0 < \alpha < 1), \]  
\[ \alpha p_\lambda^{\alpha - 1} p_\mu < (\alpha - 1)p_\lambda^\alpha + p_\mu^\alpha \quad (\alpha > 1), \]  
from which we find that the quantity in Eq. (13) satisfies

\[ G_k > \sum_\lambda p_\lambda^\alpha \langle u_\lambda | [L_k^\dagger, L_k] | u_\lambda \rangle \quad (\alpha > 0). \]  
(18)

Therefore, we obtain the following result [19]:

\[ \frac{dS_\alpha}{dt} > \sum_k c_k \langle [L_k^\dagger, L_k] \rangle_\alpha. \]  
(19)

The symbol appearing on the right-hand side stands for the escort average defined by

\[ \langle A \rangle_\alpha = \frac{\text{tr}(A\rho^\alpha)}{\text{tr}\rho^\alpha}. \]  
(20)

Thus, a positive rate is realized if the operators \( L_k \)'s are normal, i.e., \([L_k^\dagger, L_k] = 0\).

The result in Eq. (19) generalizes the one for the von Neumann entropy presented in Ref. [20], which is reproduced in the limit \( \alpha \to 1 \).

Note that the escort average is not a quantum-mechanical average unless \( \alpha \to 1 \). As shown in Refs. [21-24], like the Rényi entropy, the escort average too fails to be Lesche stable.

4. Weak invariants of quantum dissipative systems

Here, we consider a situation that the Hamiltonian of the open objective system has an explicit time dependence: \( H = H(t) \). Let \( I(t) \) be a time-dependent observable. It is referred to as a weak invariant [25] if its average \( \langle I(t) \rangle = \text{tr}(I(t)\rho(t)) \) is constant in time. Suppose \( \rho(t) \) to be a solution of the Lindblad equation in Eq. (7). Then, \( I(t) \) is a weak invariant, if it satisfies the following equation:

\[ i\frac{\partial I(t)}{\partial t} - [H(t), I(t)] - \frac{i}{2} \sum_k c_k (L_k^\dagger L_k I(t) + I(t)L_k^\dagger L_k - 2L_k^\dagger I(t)L_k) = 0. \]  
(21)

This generalizes the Lewis-Riesenfeld invariant \( I_0(t) \) [26] (see also Ref. [27]) that obeys the equation:

\[ i\frac{\partial I_0(t)}{\partial t} - [H(t), I_0(t)] = 0. \]  
(22)

Henceforth, \( I_0(t) \) satisfying Eq. (22) is referred to as a strong invariant.

A crucial difference between strong and weak invariants is that the eigenvalues of a strong invariant are constant in time, whereas those of a weak invariant are not.

A weak invariant is of physical relevance. For example, it is known [28-30] that there exists a process peculiar in quantum thermodynamics called an isoenergetic process, along which the internal energy is kept constant. Such a process is different from an isothermal process because of the quantum-mechanical violation of the law of equipartition of energy. If an isoenergetic process
is examined in the framework of finite-time quantum thermodynamics, then the time-dependent Hamiltonian is a weak invariant.

Strong invariants of the Lewis-Riesenfeld type have widely been applied to diverse problems in the literature. Examples include constructions of the coherent and squeezed states [31-34], geometric phases [35-37], nonstationary quantum field theory [38,39], fermions [40], quantum computation [41] and third-quantized cosmology [42].

The Lewis-Riesenfeld invariant is best known for the harmonic oscillator with the time-dependent frequency, the Hamiltonian of which reads

\[ H(t) = \frac{1}{2} p^2 + \frac{1}{2} \omega^2(t) x^2, \]  

provided that the mass has been set equal to unity for the sake of simplicity. The Lewis-Riesenfeld invariant associated with this Hamiltonian is given by

\[ I_0(t) = \frac{1}{2} \left[ (\sigma_0 p - \dot{\sigma}_0 x)^2 + \left( \frac{x}{\sigma_0} \right)^2 \right], \]  

where \( \sigma_0 = \sigma_0(t) \) is a c-number real quantity satisfying the following auxiliary equation:

\[ \ddot{\sigma}_0 + \omega^2(t) \sigma_0 = \frac{1}{\sigma_0^3}, \]  

where the overdots denote time derivatives: \( \dot{\sigma}_0 = d\sigma_0/dt, \ddot{\sigma}_0 = d^2\sigma_0/dt^2 \). It is then straightforward to ascertain that \( I_0(t) \) in Eq. (24) satisfies Eq. (22).

To generalize the strong invariant \( I_0(t) \) to the weak invariant of the time-dependent damped harmonic oscillator, we consider the following single Lindbladian operator:

\[ L \equiv L_1 = K_1 + a(t) K_2 + b(t) K_3. \]  

Here, \( K_i \)'s are given by \( K_1 = p^2/2, K_2 = x^2/2 \) and \( K_3 = (px + xp)/2 \) that satisfy the commutation relations: \( [K_1, K_2] = -i K_3, [K_2, K_3] = 2i K_2, [K_3, K_1] = 2i K_1, \) which is isomorphic to the \( su(1,1) \) Lie algebra. \( a(t) \) and \( b(t) \) are c-number real quantities to be discussed below. A possible factor of \( K_1 \) is absorbed into \( c \equiv c_1(t) \) in Eq. (7). Since \( L \) in Eq. (26) is Hermitian, Eqs. (7) and (21) become

\[ i \frac{\partial \rho}{\partial t} = [H(t), \rho] - \frac{i}{2} c(t) [L, [L, \rho]], \]  

\[ i \frac{\partial I(t)}{\partial t} - [H(t), I(t)] - \frac{i}{2} c(t) [L, [L, I(t)]] = 0, \]

respectively, where \( H(t) \) is the Hamiltonian given in Eq. (23).

The idea proposed in Ref. [25] is to require the classical equation of motion of the damped harmonic oscillator to hold as the expectation value:

\[ \frac{d^2 \langle x \rangle}{dt^2} + 2\kappa(t) \frac{d \langle x \rangle}{dt} + \Omega^2(t) \langle x \rangle = 0. \]  

(29)

Clearly, there exists a nontrivial point behind this requirement. In classical theory, the friction term is indivisibly connected with an external noise term, usually in conformity with the fluctuation-dissipation relation. In the case of the linear system, the expectation value satisfies the equation that is similar to Eq. (29). A possible interpretation of Eq. (29) is that
what corresponds to the noise may be the combination of the quantum fluctuations and the environmental effects.

Now, from Eq. (27) with Eqs. (23) and (26), the friction coefficient and the (modulated) frequency are found to be expressed as follows:

\[ \kappa(t) = \frac{1}{2} c(t) \left[ a(t) - b^2(t) \right], \] (30)
\[ \Omega^2(t) = \omega^2(t) + \kappa^2(t) + \dot{\kappa}(t). \] (31)

The nonnegativity condition may be imposed on these quantities. The weak invariant satisfying Eq. (28) is found to have the form

\[ I(t) = \frac{1}{2} \left[ (\sigma p - \dot{\sigma} x)^2 + \left( \frac{x}{\sigma} \right)^2 \right]. \] (32)

This is formally identical to Eq. (24). However, the \( c \)-number quantity \( \sigma = \sigma(t) \) here satisfies

\[ \ddot{\sigma} - \kappa(t)\dot{\sigma} + \omega^2(t)\sigma = \frac{1}{\sigma^3}, \] (33)

which is in contrast to Eq. (25). \( c(t), a(t) \) and \( b(t) \) are related to \( \sigma(t) \) as follows:

\[ c(t) = \frac{8\kappa\sigma^4}{(\dot{\sigma}^2 + \frac{1}{\sigma^4})}, \] (34)
\[ a(t) = \frac{1}{2} \left( \frac{\ddot{\sigma}}{\sigma} \right)^2 + \frac{1}{\sigma^4}, \] (35)
\[ b(t) = -\frac{\dot{\sigma}}{2\sigma}. \] (36)

It should be noted that the friction terms in Eqs. (29) and (33) have the opposite signs. Thus, existence of the weak invariant is linked with such a time reversal structure.

5. Concluding remarks

In this article, we have made a short review of a couple of recent topics in quantum theory of Markovian open systems, i.e., time evolution of the Rényi entropy and weak invariants.

While this article has been under preparation, our attention has been drawn to Ref. [43]. There, the authors examine time evolution of the Rényi entropy for characterizing (non-) Markovianity of quantum subdynamics.

Clearly, weak invariants can also be defined for classical systems. For example, an weak invariant associated with the Fokker-Planck equation and its application to an econophysical problem have recently been discussed in Ref. [44]. A further investigation along this line is in progress.

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