Growing fluctuation of quantum weak invariant and its connection to dissipation

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\textbf{Abstract} The concept of weak invariants has recently been introduced in the context of conserved quantities in finite-time processes in nonequilibrium quantum thermodynamics. A weak invariant itself has a time-dependent spectrum, but its expectation value remains constant under time evolution defined by a relevant master equation. Although its expectation value is thus constant in time by definition, its fluctuation is not. Here, time evolution of such a fluctuation is studied. It is proved that if the subdynamics is given by a completely positive map, then the fluctuation of the associated weak invariant does not decrease in time. As an illustrative example, the weak invariant associated with the Lindblad equation is discussed. The result shows how dissipation and the growth rate of the fluctuation are interrelated.
Although studies of open quantum systems have a long tradition [1], they seem to be at the stage of new importance today. An integral part of the reasons behind this fact may be due to rapidly-developing quantum thermodynamics [2,3] and its fundamental relevance to quantum information, quantum computation, nanoscience, and so on. A classical system treated by equilibrium thermodynamics is basically described by a set of dynamical/thermodynamical variables. In quantum thermodynamics, on the other hand, not only dynamical variables but also the Hilbert space are needed. This double structure can lead to diverse concepts of baths. Examples often discussed in the literature are the dephasing bath [4] and the energy bath [5] that have no classical counterparts. Their roles are realization of decoherence and to energy transfer [6,7], respectively. However, a situation somewhat analogous to such a double structure appears also in classical thermodynamics in the nonequilibrium regime since the kinetic approach contains both variables and distributions, as mentioned in the subsequent discussion.

Conservations of quantities or variables characterize thermodynamic processes such as the isothermal, isentropic, isenergetic, isochoric, and isobaric processes. Among these, the isenergetic process clearly stands out, since it is connected to the energy bath mentioned above. Along this process, the expectation value of the subsystem Hamiltonian as the internal energy is kept constant [8,9]. It is essential to note that, in quantum thermodynamics, it is different from the isothermal process because of the quantum-mechanical violation of the law of equipartition of energy. Expansion of size of the subsystem shifts the spectrum of the Hamiltonian lower, but energy transfer from
the energy bath can compensate it, for example. Thus, the isenergetic process highlights in a peculiar manner how quantum thermodynamics can widen the view of traditional concepts in classical thermodynamics.

The concept of weak invariants has been introduced in connection to this quantum thermodynamic background [10]. A time-dependent observable is said to be a strong invariant if its spectrum does not depend on time. A celebrated example is the Lewis-Riesenfeld invariant associated with the unitary dynamics [11], which will be mentioned later. On the other hand, a time-dependent observable is referred to as a weak invariant if its spectrum varies in time but its expectation value is conserved [10]. Recently, it has also been shown that a weak invariant can be interpreted as the Noether charge in the action principle for kinetic theory [12,13].

The purpose of the present work is as follows. By definition, the expectation value of a weak invariant is kept constant in time. However, its fluctuation may not. Here, the fluctuation of a quantum weak invariant is discussed. This issue may particularly be relevant to small systems, in which the effects of fluctuations are nonnegligible. It is shown that the fluctuation of a quantum weak invariant monotonically grows in time. For this purpose, the weak invariant associated with the Lindblad equation is considered, and the relation between dissipation and the growth rate of the fluctuation and is derived. Then, a general proof is presented for the subdynamics represented by a completely positive map.

Before discussing a quantum weak invariant, let us briefly look at a classical weak invariant associated with the Fokker-Planck equation [14]:

$$\frac{\partial P}{\partial t} = -\sum_{i=1}^{N} \frac{\partial (K_i P)}{\partial x_i}$$
\[ + \sum_{i,j=1}^{N} \frac{\partial^2 (D_{ij} P)}{\partial x_i \partial x_j}, \text{ where } P(x,t)d^N x \text{ is the probability of finding the } N\text{-tuple of the variables } x=(x_1, x_2, \ldots, x_N) \text{ in the region } [x_1, x_1+dx_1] \times [x_2, x_2+dx_2] \times \ldots \times [x_N, x_N+dx_N] \text{ at time } t. \text{ Both } K_i \text{'s in the drift term and the } N \times N \text{ diffusion matrix } D=(D_{ij}) \text{ may depend on } x \text{ and } t. \text{ In particular, } D \text{ should be a symmetric and positive definite matrix. A weak invariant associated with this kinetic equation is a quantity, } J(x,t) \text{, satisfying } \frac{\partial J}{\partial t} + \sum_{i=1}^{N} K_i \frac{\partial J}{\partial x_i} + \sum_{i,j=1}^{N} D_{ij} \frac{\partial^2 J}{\partial x_i \partial x_j} = 0. \]

Under the assumption that the probability distribution and its derivatives vanish sufficiently rapid in the limit \(|x| \to \infty\), the expectation value of the weak invariant, \[ \mathcal{J} = \int d^N x J(x,t) P(x,t) \] with the domain of integration being the whole \(N\)-dimensional space, is shown to be conserved in time: \(d \mathcal{J}/dt = 0\). Since boundary conditions do not have to be imposed on the weak invariant, in general, there is freedom in its choice, depending on problems of interest. For example, if a multivariate polynomial of \(x_i\)’s with time-dependent coefficients is chosen as \(J(x,t)\), then constancy of \(\mathcal{J}\) gives information on how the moments and correlations between the variables evolve in time in a specific way. Although the expectation value is conserved, the variance, \((\delta J)^2 = \mathcal{J}^2 - (\mathcal{J})^2\), depends on time. In fact, from the Fokker-Planck equation and the equation for the weak invariant given above, we obtain the multivariate generalization of the result given in Refs. [13,15]:

\[ d(\delta J)^2 / dt = \frac{d \mathcal{J}^2}{dt} = 2 \sum_{i,j=1}^{N} D_{ij} (\frac{\partial J}{\partial x_i})(\frac{\partial J}{\partial x_j}) \], showing that the
fluctuation of the classical weak invariant associated with the Fokker-Planck equation monotonically grows in time. It is worth noting that the drift term does not contribute to the growth rate of the fluctuation of the weak invariant.

Now, let us discuss a quantum weak invariant and time evolution of its fluctuation. The master equation we consider here is the Lindblad equation [16-18], which is given by

$$i \frac{\partial \rho}{\partial t} = [H, \rho] - i \sum_n c_n (L_n^\dagger L_n \rho + \rho L_n^\dagger L_n - 2 L_n \rho L_n^\dagger),$$

(1)

where $\rho$ is the density matrix describing the quantum state of the subsystem under consideration, $H$ is the subsystem Hamiltonian, and $c_n$’s are positive $c$-number coefficients. $H$, the Lindbladian operators $L_n$’s, and $c_n$’s may explicitly depend on time. Here and hereafter, $\hbar$ is set equal to unity. The second term on the right-hand side is referred to as the dissipator. Equation (1) is known to be the most general linear Markovian equation that preserves positive semidefiniteness of the density matrix. A weak invariant, $I(t)$, associated with Eq. (1) is an observable satisfying

$$\frac{\partial I}{\partial t} + i [H, I] - \sum_n c_n (L_n^\dagger L_n I + I L_n^\dagger L_n - 2 L_n^\dagger I L_n) = 0.$$  

(2)

A couple of comments on this equation are in order. Firstly, this equation remains unchanged under the shift: $I(t) \rightarrow I(t) + a \mathbb{1}$, where $a$ is a constant and $\mathbb{1}$ stands for the identity operator. Secondly, if the weak invariant and the Lindbladian operators commute with each other, i.e., $[L_n, I] = 0$ for all $n$, then the third term on the left-hand
side vanishes, and Eq. (2) becomes reduced to \( \frac{\partial I}{\partial t} + i[H, I] = 0 \), which is the equation for the Lewis-Riesenfeld strong invariant associated with the time-dependent Hamiltonian [11]. Therefore, it is essential for our purpose to impose the condition that the weak invariant does not commute with the Lindbladian operators.

From Eqs. (1) and (2), it follows that the expectation value, \( \langle I \rangle = \text{tr}(I(t)\rho(t)) \), is in fact conserved:

\[
\frac{d\langle I \rangle}{dt} = 0.
\] (3)

Let us discuss time evolution of the variance, \( (\Delta I)^2 = \langle I^2 \rangle - \langle I \rangle^2 \). A straightforward calculation with Eqs. (1) and (2) leads to the following result:

\[
\frac{d(\Delta I)^2}{dt} = 2 \sum_n c_n \langle [L_n, I]^+ [L_n, I] \rangle.
\] (4)

This establishes a new relation between dissipation and weak invariant. We wish to emphasize that Eq. (4) is not an inequality but an equality, in contrast to the entropy production rate [19,20]. Since the right-hand side in Eq. (4) is positive, the fluctuation of the weak invariant associated with the Lindblad equation monotonically grows in time, similarly to the case of the Fokker-Planck equation (the right-hand side does not vanish because of the basic premise that the weak invariant does not commute with the Lindbladian operators, as mentioned in the preceding paragraph). Also, we see that, analogously to the drift term of the Fokker-Planck equation, the subsystem Hamiltonian does not contribute to the growth rate of the fluctuation. In addition, it is shown in Ref. [13] that the weak invariant can be thought of as the Noether charge. In this respect, the
commutator, \([L_n, L]\), appearing in Eq. (4) is interpreted as a deformation of the Lindbladian operators through a transformation of the density matrix generated by the weak invariant.

Let us examine the result in Eq. (4) by employing an explicit example. In Ref. [10], the Lewis-Riesenfeld strong invariant of the time-dependent harmonic oscillator has been generalized to the weak invariant of the time-dependent damped harmonic oscillator. There, the time-dependent subsystem Hamiltonian is given by

\[ H(t) = K_1 + \omega^2(t) K_2, \]

where \( \omega(t) \) is the time-dependent frequency. The mass is set equal to unity for the sake of simplicity. \( K_1 \) and \( K_2 \) are the operators, which are given in terms of the momentum and position operators, \( p \) and \( x \), as \( K_1 = p^2 / 2 \) and \( K_2 = x^2 / 2 \). Together with \( K_3 = (px + xp) / 2 \), these form the \( su(1,1) \) Lie algebra:

\[
[K_1, K_2] = -i K_3, \quad [K_2, K_3] = 2i K_2, \quad [K_3, K_1] = 2i K_1.
\]

The one and only Lindbladian operator needed for the damped harmonic oscillator has turned out to be

\[ L = L_1 = a_1(t) K_1 + a_2(t) K_2 + a_3(t) K_3, \]

where \( a(t) \)'s are real \( c \)-number functions of \( t \), and thus, \( L \) is Hermitian. Since one of \( a(t) \)'s can be absorbed into the coefficient, \( c_1 = c(t) > 0 \) appearing in the Lindblad equation, \( a_1 \) may be set to unity without loss of generality. Then, it has been shown that the expectation value of the position operator satisfies the equation of motion of the damped harmonic oscillator:

\[
d^2 \langle x \rangle / dt^2 + 2 \kappa(t) d \langle x \rangle / dt + \Omega^2(t) \langle x \rangle = 0,
\]

where the friction coefficient and the
squared modulated frequency are respectively given by $\kappa(t) = c(t)\bigl[a_2(t) - a_3^2(t)\bigr]$ and $\Omega^2(t) = \omega^2(t) + \kappa^2(t) + \dot{\kappa}(t)$, where the over-dot stands for time derivative. The inequality, $a_2(t) - a_3^2(t) > 0$, must be fulfilled in order for $\kappa(t)$ to be nonnegative. Consequently, the Lindblad equation for the damped harmonic oscillator has turned out to be given as follows: $i\partial \rho / \partial t = [H(t), \rho] - i c(t) [L(t), [L(t), \rho]]$ with $L = K_1 + a_2(t) K_2 + a_3(t) K_3$. Associated with this equation, the weak invariant has been found to be of the form [10]: $I(t) = \rho^2 K_1 + (\dot{\rho}^2 + 1/\rho^2) K_2 - \rho \dot{\rho} K_3$, where $\rho = \rho(t)$ is the $c$-number function satisfying the so-called auxiliary equation: $\dot{\rho} - \kappa(t) \dot{\rho} + \omega^2(t) \rho = 1/\rho^3$. This $I(t)$, in fact, satisfies the equation for the weak invariant associated with the above-mentioned Lindblad equation: $\partial I / \partial t + i[H(t), I] - c(t) [L(t), [L(t), I]] = 0$. This naturally generalizes the Lewis-Riesenfeld strong invariant [11], which is reproduced in the vanishing friction limit $c(t) \to 0^+$. Using Eq. (4), we immediately obtain the following growth rate of the fluctuation of this weak invariant: $d (\Delta I)^2 / dt = 2 c(t) \left\{2\alpha_1 K_1 - 2\alpha_2 K_2 - \alpha_3 K_3\right\}^2$, where $\alpha$'s are $c$-number real functions of time given by $\alpha_1(t) = \rho \dot{\rho} + a_3 \rho^2$, $\alpha_2(t) = a_2 \rho \dot{\rho} + a_3 (\dot{\rho}^2 + 1/\rho^3)$, and $\alpha_3(t) = \dot{\rho}^2 + 1/\rho^2 - a_2 \rho^2$. As mentioned above, in the vanishing friction limit $c(t) \to 0^+$, the weak invariant tends to the Lewis-Riesenfeld strong invariant, and its fluctuation remains constant in time. This demonstrates how the growth of the fluctuation of the weak invariant is connected to dissipation.

Finally, let us consider a quantum weak invariant and its fluctuation within a
framework somewhat more general. Time evolution of the density matrix may be
described by a completely positive map, \( \Phi_t \), in the Kraus representation [18,21]:

\[
\Phi_t : \rho(0) \rightarrow \rho(t) = \Phi_t \left( \rho(0) \right) = \sum_k V_k(t) \rho(0) V_k^\dagger(t)
\]

(5)

with the trace-preserving condition

\[
\sum_k V_k^\dagger(t) V_k(t) = \mathbf{I},
\]

(6)

which implies that the set \( \left\{ V_k^\dagger(t) V_k(t) \right\}_k \) forms a positive operator-valued measure. By
definition, a weak invariant associated with the map in Eq. (5) satisfies

\[
\text{tr} \left[ I(t) \rho(t) \right] = \text{tr} \left[ I(0) \rho(0) \right],
\]

(7)

for any \( t > 0 \). The left-hand side in this equation is rewritten as follows:

\[
\text{tr} \left[ I(t) \rho(t) \right] = \text{tr} \left[ I(t) \Phi_t \left( \rho(0) \right) \right] = \text{tr} \left[ \Phi_t^\dagger \left( I(t) \right) \rho(0) \right].
\]

(8)

In this equation, \( \Phi_t^\dagger \) denotes the adjoint of \( \Phi_t \):

\[
\Phi_t^\dagger \left( I(t) \right) = \sum_k V_k^\dagger(t) I(t) V_k(t).
\]

(9)
Therefore, $I(t)$ is a weak invariant associated with the map, $\Phi_t$, if

$$\Phi_t^*(I(t)) = I(0)$$  \hspace{1cm} (10)

holds. A crucial point is that, because of Eq. (6), the identity operator is a fixed point of $\Phi_t^*$, i.e., $\Phi_t^*(I) = I$. Therefore, $\Phi_t^*$ is not only completely positive but also unital. On the other hand, regarding the variance, $(\Delta I)^2(t) = \text{tr}\left[I^2(t)\rho(t)\right] - \left\{\text{tr}\left[I(t)\rho(t)\right]\right\}^2$

$= \text{tr}\left[I^2(t)\rho(t)\right] - \left\{\text{tr}\left[I(0)\rho(0)\right]\right\}^2$, what to be examined is the second moment

$$\text{tr}\left[I^2(t)\rho(t)\right] = \text{tr}\left[\Phi_t^*(I^2(t))\rho(0)\right].$$  \hspace{1cm} (11)

From Kadison’s theorem for a completely positive unital map [22] and operator concave $I^2(t)$ with $I(t)$ being Hermitian, it follows that

$$\Phi_t^*(I^2(t)) \geq \left[\Phi_t^*(I(t))\right]^2 = I^2(0).$$  \hspace{1cm} (12)

Therefore, we obtain the general result

$$(\Delta I)^2(t) \geq (\Delta I)^2(0).$$  \hspace{1cm} (13)

The equality holds for unitary dynamics corresponding to the strong invariant.

In conclusion, we have shown that the fluctuation of the weak invariant associated
with the subdynamics described by a completely positive map grows, in general. We have found in the case of the Lindblad equation how the growth rate of the fluctuation is connected to dissipation.

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