Equivalence of two Bochkov-Kuzovlev equalities in quantum two-level systems

Fei Liu

School of Physics and Nuclear Energy Engineering, Beihang University, Beijing 100191, China

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We present two kinds of Bochkov-Kuzovlev work equalities in a two-level system that is described by a quantum Markovian master equation. One is based on multiple time correlation functions and the other is based on the quantum trajectory viewpoint. We show that these two equalities are indeed equivalent. Importantly, this equivalence provides us a way to calculate the probability density function of the quantum work by solving the evolution equation for its characteristic function. We use a numerical model to verify these results.

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Introduction. In the past decade, the extension of classical fluctuation relations [1–13] into a nonequilibrium quantum regime has attracted intensive interest [1,14–32]. In the literature, the quantum measurement [15,17,20,21,27] and the quantum trajectory in Hilbert space [19,24,28–30,33–36] are two widely used fundamental concepts. As an alternative to those two concepts, very recently, Chetrite and Mallick [37] and we [38] showed that, in the isolated Hamiltonian system and some quantum Markovian master equations (QMMEs) [34,39], the quantum work equalities [1,6] can be derived based on the time-reversal and quantum Feynman-Kac formulas. In contrast with the conventional work equalities written as the statistical average of exponential functions [19,24,28–30], which we name the c-number equalities, these recently obtained equalities, which are named the q-number equalities, are remarkable analogies with their classical counterparts [37,38].

Even so, in the case of the QMMEs, the exact relationship between those two concepts, very recently, Chetrite and Mallick [37] and we [38] showed that, in the isolated Hamiltonian system and some quantum Markovian master equations (QMMEs) [34,39], the quantum work equalities [1,6] can be derived based on the time-reversal and quantum Feynman-Kac formulas. In contrast with the conventional work equalities written as the statistical average of exponential functions [19,24,28–30], which we name the c-number equalities, these recently obtained equalities, which are named the q-number equalities, are remarkable analogies with their classical counterparts [37,38].

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where $L^{\ast}_r$ is the dual of $L_r$ [34]. We also introduce the superoperator $\mathcal{W}$, Its action on an operator is a multiplication from the right-hand side of the operator. Using the celebrated Dyson series, Eq. (8) has the following formal solution [37,51]:

$$R(t',T) = \left[ G^{\ast}(t',T) + \sum_{n=1}^{\infty} \int_{0}^{T} dt_1 \cdots \int_{t_{n-1}}^{T} dt_n \prod_{i=1}^{n} G^{\ast}(t_{i-1},t_i) \mathcal{W}_i G^{\ast}(t_n,T) \right] R(T,T),$$

(10)

where $G^{\ast}(t_1,t_2) = T_+ \exp[\int_{t_1}^{t_2} dt L^{\ast}_r] (t_1 < t_2)$ is the adjoint propagator of the system, and $T_+$ denotes the antichronological time-ordering operator. Notice that $G^{\ast}(t_1,t_2)(I) = I$ [34].

Equation (7) has a trivial property, i.e., the traces of its two sides are 1. Hence, substituting Eq. (10) and letting $t' = 0$, we obtain the $q$-number BKE:

$$1 = \text{Tr}[R(0,T)\rho_0] = 1 + \int_{0}^{T} dt_1 \text{Tr} \left[ \left\{ i\hbar [H_1(t_1),\rho_0] \right\}^{-1} G(t_1,0)\rho_0 \right] + \cdots = \left( T_+ \exp \left[ \int_{0}^{T} dt i\hbar H_1(t)\rho_0 \right] \right) \rho_0^{-1} \rho_0, \quad (11)$$

In the quantum optics, these jumps appear as an absorption or emission of a photon [33–36]. Hence, the corresponding energy could be physically interpreted as heat absorbed or released by the system from or to the heat bath [19,23,24,28,30]. By measuring the energy of the TLS at the beginning time ($\epsilon_n$) and ending time ($\epsilon_m$) while recording the number $N_+ (N_-)$ of the jumps to $|g\rangle$ ($|e\rangle$) along a quantum trajectory, we define the work done by the driving field on the TLS as

$$W = \epsilon_n - \epsilon_m + \alpha \hbar \int_{0}^{T} dN_+ - \alpha \hbar \int_{0}^{T} dN_-, \quad (13)$$

where $dN_+$ and $dN_-$ are the increments of these two types of jumps. We remind the reader that the first two terms are the energy eigenvalues of the free Hamiltonian $H_0$ instead of the total Hamiltonian. With the above notations, we give the $c$-number BKE for the quantum work (13):

$$1 = \sum_{m,n} p_m(0) \int_{0}^{T} \cdots \int_{t_{n-1}}^{T} \prod_{i=1}^{N} dt_i \sum_{\gamma_1} \cdots \sum_{\gamma_N} \times \left[ \prod_{i=1}^{N} \langle n | \mathcal{L}_N | m \rangle \right] e^{-\beta W} = E[e^{-\beta W}], \quad (14)$$

where $p_m(0) = \exp(-\beta \epsilon_m)/\text{Tr}[\exp(-\beta H_0)]$ is the initial probability of the TLS at the eigenstate with the energy $\epsilon_m$; the whole term inside the square brackets of the first equation is the probability density of observing a quantum trajectory that starts from the eigenstate $|m\rangle$, with a jump occurring at time $t_i$ with type $P_i$ that equals $\sigma_+$ or $\sigma_-$ with the jump rate $\gamma_1$ or $\gamma_1$ ($i = 1, \ldots, N$), and ends in the eigenstate $|n\rangle$ at the final time $T$; and

$$\mathcal{L}_N = U(T,t_N)P_N \cdots U(t_2,t_1)P_1 U(t_1,0)$$

(15)

is the time evolution operator of the whole trajectory [34]. We specifically use the notation $E[\cdots]$ to denote the average in the $c$-number equality. Proof of the equality will be seen shortly.
Equivalence of the two BKEs. Although we name Eq. (11) the BKE, its physical relevance is not obvious. We do not see from the abstract equality what the work is and whether the second law of thermodynamics is implied. It is quite different from the c-number BKE (14). At first glance, these two equalities appear so distinct. However, we will show that it is only superficial. Before the summation over \( m \), Eq. (14) can be rewritten as

\[
p_m(0) \sum_{N=0}^{\infty} \int_0^T \cdots \int_{s_{k-1}}^{s_k} d\gamma_1 \cdots \int_{s_N}^{s_{N+1}} d\gamma_N \left[ \prod_{i=1}^N \gamma_i |m| \mathcal{E}_N^i |n| \right]^2 e^{-\beta W} e^{-\beta \hbar (\omega N_e - \omega N)}
\]

\[
= \langle m| | m \rangle^{-1} \sum_{N=0}^{\infty} p_m(0) \int_0^T \cdots \int_{s_{k-1}}^{s_k} d\gamma_1 \cdots \int_{s_N}^{s_{N+1}} d\gamma_N \sum_{n=0}^{N} \prod_{i=1}^N \gamma_i \mathcal{L}_N |\Theta|n| \Theta^{-1} | \mathcal{L}_N^\dagger | \Theta | m \rangle
\]

where \( \tilde{\gamma}_i = y_i \), \( \gamma_i = y_i + s_i + \imath N + 1 - i = T \),

\[
\mathcal{L}_N = \tilde{U}(T, s_N) P_1 \cdots \tilde{U}(s_2, s_1) P_1 \tilde{U}(s_1, 0)
\]

is the time evolution operator of the reversed quantum trajectory, and \( \tilde{U}(s, s_1) \) is analogous to the previous \( U(t, t_1) \) except that the Hamiltonian therein is replaced by \( H_0 + \tilde{H}(s) \). The last exponential term in the first line of Eq. (16) is the consequence of the detailed balance condition (3), and the final equation is due to the well-established relationship between the density matrix and the quantum trajectory [34,36]. Comparing Eq. (7) with Eq. (16), we immediately see that the whole expression after \( p_m(0) \) is just \( \langle m|R(0, T)|m \rangle \) on the left-hand side of the latter equation. Therefore, we prove that the c-number and q-number BKEs are exactly equivalent.

An alternative proof of this equivalence that does not depend on the time-reversal explanation is to do series expansions for these two BKEs in terms of \( \beta \). We then compare their respective coefficients of the different orders of \( \beta \). For the c-number BKE, the expansion is simply

\[
1 = 1 - E[W] \beta + \frac{1}{2} E[W^2] \beta^2 \cdots .
\]

Using the facts that \( E[dn_{+}] = y_1 \Gamma_{\theta} \rangle |T \Gamma_{\theta} \rangle |T \rangle \) and \( E[dn_{-}] = y_1 \Gamma_{\theta} \rangle |T \Gamma_{\theta} \rangle |T \rangle \) [34,36], where \( t \) is the time of nonvanishing \( dN_{\pm} \), we rewrite the first moment of the work (13) as (see the Supplemental Material [55])

\[
E[W] = \int_0^T dt_1 \int_0^T dt_2 \left[ \left\{ i \hbar \langle H_1(t_2), H_0 \rangle \right\} \left\{ i \hbar \langle H_1(t_1), H_0 \rangle \right\} \right] - \frac{1}{2} \int_0^T dt_1 \left\{ \frac{i}{\hbar} \langle H_1(t_1), H_0 \rangle, H_0 \rangle \right\}
\]

Because the left-hand side is the average work and the first integration in the first equation represents a change of average energy of the TLS during the whole process, we may interpret the second integration in the same equation as the absorbed average heat from the heat bath. Hence, Eq. (19) is just the first law of thermodynamics. Using the Jensen’s inequality, we surely have the second law of thermodynamics, \( E[W] \geq 0 \). A more complex case is the second moment. Using the three crucial identities below [56],

\[
E[dN_{+} dN_{-}'] = y_1 y_1' \langle T \Gamma_{\theta} \rangle |T \Gamma_{\theta} \rangle |T \rangle \theta(t - t') + y_1 y_1' \langle T \Gamma_{\theta} \rangle |T \Gamma_{\theta} \rangle |T \rangle \theta(t' - t),
\]

\[
E[dN_{-} dN_{-}'] = y_1 y_1' \langle T \Gamma_{\theta} \rangle |T \Gamma_{\theta} \rangle |T \rangle \theta(t - t') + y_1 y_1' \langle T \Gamma_{\theta} \rangle |T \Gamma_{\theta} \rangle |T \rangle \theta(t' - t),
\]

\[
E[dN_{+} dN_{-}'] = y_1 y_1' \langle T \Gamma_{\theta} \rangle |T \Gamma_{\theta} \rangle |T \rangle \theta(t - t') + y_1 y_1' \langle T \Gamma_{\theta} \rangle |T \Gamma_{\theta} \rangle |T \rangle \theta(t' - t)dtdt',
\]

where \( t (t') \) is the time of nonvanishing \( dN_{\pm} \) (\( dN_{\pm} \)), and, by performing a careful calculation, we obtain

\[
\frac{1}{2} E[W^2] = \int_0^T dt_1 \int_0^T dt_2 \left\{ \frac{i}{\hbar} \langle H_1(t_2), H_0 \rangle \right\} \left\{ \frac{i}{\hbar} \langle H_1(t_1), H_0 \rangle \right\} - \frac{1}{2} \int_0^T dt_1 \left\{ \frac{i}{\hbar} \langle H_1(t_1), H_0 \rangle, H_0 \rangle \right\}.
\]

First, we may apply Eqs. (19) and (23) to calculate the first two moments of the work by analytically or numerically solving the master equations rather than by doing the quantum jump simulation. Compared with the latter, the former is exact and involves no sampling errors. As an illustration, we recalculate these moments for the TLS model in Ref. [30], where \( H_1(t) = \lambda_0 \sin(\omega t)(\sigma_+ + \sigma_-) \); see Fig. 1. The simulation data are also...
be $\Phi(u)$, where $u$ is the real number, we easily see that

$$\Phi(u) = E[e^{iuW}] = \frac{\text{Tr}[K(0, T; u)\rho_0]}{\rho_0},$$

if the introduced operator $K(t', T; u)$ satisfies the evolution equation given by

$$\partial_{t'} K(t', T; u) = -L'_T K(t', T; u) - K(t', T; u)$$

$$\times \frac{i}{\hbar} [H(t'), e^{iuH_0}] e^{-iuH_0},$$

$$K(T, T; u) = I.$$  (25)

By numerically solving the above equation and performing an inverse Fourier transform of $\Phi(u)$, the pdf of the work is then obtained. The inset of Fig. 1 is an example. We see that our calculation excellently agrees with the simulation data [30].

Conclusion. In this work, we present two kinds of BKEs in the quantum TLS driven by the field and we prove their equivalence. Moreover, an efficient way of calculating the characteristic function of the quantum work is revealed. So far, our discussions are limited to these specific QMMEs where the driven field is so weak that their dissipations can be treated as time independent. Extending the current idea into the more general cases, e.g., the master equations with time-dependent dissipations, shall be very intriguing. We expect that some of them would be related to the quantum Jarzynski equality. This study is underway.

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[54] Hekking and Pekola should have first presented the $c$-number BKE [30]. However, they claimed that they verified the quantum Jarzynski equality. Compared with what we did in this work, they used a different and relatively complex method.
[55] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevE.89.042122 for the proof of Eqs. (19) and (23), the details of calculating $K(t, T; u)$ for the TSL model in Ref. [30], and the general structure of the QMMEs about which we are concerned here.
[56] These equations are the generalizations of Eq. (4.50) in the book of Wiseman and Milburn [36].