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

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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, extending classical fluctuation relations [1–13] into nonequilibrium quantum regime is attracting 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 (QMME) [34, 46], 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 statistical average of exponential functions [19, 24, 28–30], which we name them the c-number equalities, the newly obtained equalities that 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 of the q-number and c-number equalities, and whether the q-number equalities are useful besides their forms have not been seriously considered. In this Rapid communication, we use a driven quantum two-level system (TLS) with dissipation to prove that, the q-number and the c-number Bochkov-Kuzovlev equalities (BKE) are indeed equivalent for a specific class of QMMEs. An important consequence of this investigation is that we find an efficient way to calculate the probability density function (pdf) of the quantum work for these systems without doing the quantum jump simulation [34, 36].

Driven quantum two-level system. The TLS has a free Hamiltonian $H_0 = \hbar \omega \sigma_z / 2$. Initially, the system is in the thermal state $\rho_0 = \exp(-\beta H_0) / \text{Tr}[\exp(-\beta H_0)]$ and $\beta$ is the inverse temperature of the surrounding heat reservoir. After time $0$, a driving field is applied on the system up to the final time $T$. During the whole process, we assume that the evolution equation of the reduced density matrix of the system $\rho(t)$ is

$$\partial_t \rho(t) = L_t \rho(t) = -\frac{i}{\hbar} [H_0 + H_1(t), \rho(t)] + D[\rho(t)], \quad (1)$$

where $H_1(t)$ is the interaction energy of the system and the driving field and we do not need to specify its concrete expression now. The time-independent term $D$ represents the dissipation due to the interaction between the TLS and the heat bath, which is

$$D[\rho(t)] = \gamma_\downarrow (\sigma_- \rho \sigma_+ - \frac{1}{2} \{\rho, \sigma_+ \sigma_-\}) + \gamma_\uparrow (\sigma_+ \rho \sigma_- - \frac{1}{2} \{\rho, \sigma_- \sigma_+\}), \quad (2)$$

where the two damping rates satisfy the detailed balance condition $\gamma_\downarrow = \gamma_\uparrow \exp(-\beta \hbar \omega)$. \quad (3)

This condition ensures that the system relaxes to the thermal state $\rho_0$ if we switch off $H_1(t)$. Equation (1) represents a class of QMMEs, in which the coupling of the driving field to the system and the bath is weak [34, 46]. We must point out that, the model is distinct from those in previous work [19, 24, 28, 34]: if one fixes the driving field at some value, the TLS may relax to some steady state but generally not to the thermal state $\propto \exp[-\beta (H_0 + H_1)]$. The superoperator $D$ possesses an important property $[47]$:

$$D[A\rho_0] = D^* [A] \rho_0, \quad (4)$$

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where the dual of $D$ is
\[
D^*[A] = \gamma_0(\sigma_+ A \sigma_- - \frac{1}{2}\{A, \sigma_+ \sigma_-\}) + \gamma_1(\sigma_- A \sigma_+ - \frac{1}{2}\{A, \sigma_- \sigma_+\}).
\] (5)

**Q-number BKE.** Following the spirit of establishing the classical work equalities \[45 \sim 50\], we first introduce the time-reversed process $\dot{\rho}(s)$ of Eq. (1). Its master equation is
\[
\partial_s \dot{\rho}(s) = \tilde{L}_s \dot{\rho}(s) = -\frac{i}{\hbar}[H_0 + \tilde{H}_1(s), \dot{\rho}(s)] + D[\dot{\rho}(s)],
\] (6)

where $H_0$ is time-reversible, $\tilde{H}_1(s) = \Theta H_1(t') \Theta^{-1}$ with $t' = T - s$, and $\Theta$ is time-reversal operator. We specifically set up the initial condition of the reversed process to be $\rho_0$. The next step is to obtain a solution for the operator $R(t', T)$ which is defined as
\[
\dot{\rho}(s) = \Theta R(t', T) \rho_0 \Theta^{-1}.
\] (7)

$R(t', T)$ indicates the deviation of the perturbed system from the equilibrium state $\rho_0$. Obviously, $R(T, T)$ is the identity operator $I$. Substituting Eq. (7) into Eq. (6) and using the relationship (4), we obtain an equation of motion for $R(t', T)$ with respect to $t'$:
\[
\partial_s R(t', T) = -L_*^n R(t', T) - R(t', T) \frac{i}{\hbar}[H_1(t'), \rho_0 \rho_0^{-1}] - L_*^n R(t', T) - W_t R(t', T),
\] (8)

where $L_*^n$ is the dual of $L^n$. We also introduced the superoperator $W_t$. 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 \[34 \sim 51\]:
\[
R(t', T) = [G^*(t', T) + \sum_{n=1}^{\infty} \int_0^T dt_1 \cdots \int_0^{t_{n-1}} dt_n \prod_{i=1}^n G^*(t_{i-1}, t_i) W_{t_i} G^*(t_n, T)] R(T, T),
\] (9)

where $G^*(t_1, t_2) = \mathcal{T}_+ \exp[\int_{t_1}^{t_2} dt L_*^n]$ ($t_1 < t_2$) is the adjoint propagator of the system, and $\mathcal{T}_+$ denotes the antichronological time-ordering operator. Notice that $G^*(t_1, t_2)(I) = I$ \[34\].

Equation (7) has a trivial property, i.e., the traces of its both sides being 1. Hence, substituting Eq. (10) and letting $t' = 0$, we obtain the q-number BKE:
\[
1 = \text{Tr}[R(0, T) \rho_0] = 1 + \int_0^T dt_1 \text{Tr}[\frac{i}{\hbar}[H_1(t_1), \rho_0 \rho_0^{-1}] G(t_1, 0)(\rho_0)] + \cdots
\]
\[
= 1 + \int_0^T dt_1 \langle \frac{i}{\hbar}[H_1(t_1), \rho_0 \rho_0^{-1}] \rangle + \cdots
\]
\[
= ( \mathcal{T}_+ \text{exp}(\int_0^T dt \frac{i}{\hbar}[H_1(\tau), \rho_0 \rho_0^{-1}]) ),
\] (11)

where $G(t_2, t_1) = \mathcal{T}_- \exp[\int_{t_1}^{t_2} dt L_\tau]$ is the system’s propagator from time $t_1$ to $t_2$, and $\mathcal{T}_-$ denotes the chronological time-ordering operator. We have used the property $\text{Tr}[G^*(t_1, t_2)(A)B] = \text{Tr}[AG(t_2, t_1)(B)]$ \[34\]. We denote the form of the right-hand side of Eq. (11) the quantum Feynman-Kac formula \[37 \sim 38\]. We must remind the reader that the notation $(\cdots)$ or the “average” above is a shorthand of the multi-time correlation functions of the operators \[34\]. In the absence of the dissipation term $D$, Eq. (11) reduces into the quantum BKE for the isolated Hamiltonian system \[26 \sim 38\]. Moreover, if we interpret $-i[\cdots]/\hbar$ as Poisson bracket, the density matrices as distribution functions, and the propagators under classical meaning, Eq. (11) then becomes the classical BKE \[1 \sim 51 \sim 52 \sim 53\]. It is worthy emphasizing that the concrete formulas of $H_0$ and $D$ are not involved in the above discussion.

**C-number BKE.** On the basis of the theory of quantum jump trajectory, we may obtain an alternative quantum BK equality \[54\]. Since the basic idea and techniques have been given previously \[19 \sim 24 \sim 30\], here we only present the
We prove that the c-number and q-number BKEs are exactly equivalent. Specifically, the whole expression after the consequence of the detailed balance condition (4), and the final equation is due to the well-established relationship $H$ except that the Hamiltonian therein is replaced by $\tilde{H}$. Occasionally, this evolution is interrupted by a stochastic jump to one of the states: $\sigma_+\psi(t)/||\sigma_+\psi(t)||^2$ and $\sigma_-\psi(t)/||\sigma_-\psi(t)||^2$. For the TLS these are the excited state $|\epsilon\rangle$ and ground state $|g\rangle$, respectively. In the quantum optics, these jumps appear an absorption or emission of a photon. Hence, the corresponding energy could be physically interpreted as heat absorbed or released by the system from or to the heat bath. 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 $|\epsilon\rangle$ ($|g\rangle$) along a quantum trajectory, we define the work done by the driving field on the TLS as

$$ W = \epsilon_n - \epsilon_m - \omega \hbar \int_0^T dN_+ + \omega \hbar \int_0^T dN_-, $$

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]:

$$ 1 = \sum_{m,n} p_m(0) \sum_{N=0}^{\infty} \int_0^T \cdots \int_{t_{N-1}}^T \prod_{i=1}^N dt_i \prod_{\gamma_i} \sum_{\gamma_N} \prod_{\gamma_i=1}^N \langle n | L_N | m \rangle^2 \ e^{-\beta W} = E[e^{-\beta W}], $$

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 $|m\rangle$, occurs jump at time $t_i$ with type $P_i$ that equals $\sigma_+$ or $\sigma_-$ with the jump rate $\gamma_i = \gamma_+$ or $\gamma_-$ ($i=1, \ldots, N$), and ends in the eigenstate $|n\rangle$ at the final time $T$, and

$$ L_N = U(T, t_N)P_N \cdots U(t_2, t_1)P_1 U(t_1, 0) $$

is the time evolution operator of the whole trajectory. 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 [13]. At first glance, these two equalities appear so distinct. However, we will show that it is only superficial. Before the summation over $m$, Eq. (13) can be rewritten as

$$ p_m(0) \sum_n \sum_{N=0}^{\infty} \int_0^T \cdots \int_{t_{N-1}}^T \prod_{i=1}^N dt_i \prod_{\gamma_i} \sum_{\gamma_N} \prod_{\gamma_i=1}^N \langle n | L_N^\dagger | m \rangle^2 \ e^{-\beta W} e^{-\beta (\hbar \omega N_+ - \hbar \omega N_-)} $$

$$ = \langle m | \Theta^{-1} \sum_n p_n(0) \sum_{N=0}^{\infty} \int_0^T \cdots \int_{s_{N-1}}^T \prod_{i=1}^N ds_i \prod_{\gamma_i} \sum_{\gamma_N} \prod_{\gamma_i=1}^N \tilde{\gamma}_N \Theta | n \rangle \langle n | \Theta^{-1} \tilde{L}_N^\dagger \Theta | m \rangle $$

$$ = \langle m | \Theta^{-1} \tilde{\rho}(T) \Theta | m \rangle, $$

where $\tilde{\gamma}_i = \gamma_+, \tilde{\gamma}_i = \gamma_-$, $s_i + t_{N+1-i} = T$.

$$ \tilde{L}_N = \tilde{U}(T, s_N)P_N^\dagger \cdots \tilde{U}(s_2, s_1)P_1^\dagger \tilde{U}(s_1, 0) $$

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 $H_0 + \dot{H}_1(s)$. The last exponential term in the first line of Eq. (16) is the consequence of the detailed balance condition [38], and the final equation is due to the well-established relationship between the density matrix and the quantum trajectory [33, 34]. 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

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

(18)

Using the facts that $E[dN_+] = \gamma_+ \text{Tr}[\sigma_+\sigma_+\rho(t)]dt$ and $E[dN_-] = \gamma_+ \text{Tr}[\sigma_+\sigma_+\rho(t)]dt$ \[34, 36\], where $t$ is the time of non-vanishing $dN_{\pm}$, we rewrite the first moment of the work \[13\] as (see the Supplemental Material)

$$E[W] = \int_0^T dt_1 \frac{d}{dt_1} \text{Tr}[H_0\rho(t_1)] - \int_0^T dt_1 \text{Tr}[D^*\rho(t_1)] = \int_0^T dt_1 \langle \frac{i}{\hbar} [H_1(t_1), H_0]\rangle .$$

(19)

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 \[55, \]

$$E[dN_+dN_-] = \{ \gamma_+^2 \text{Tr}[\sigma_+\sigma_+G(t,t')(\sigma_+\rho(t')\sigma_+)] + \delta(t-t')\gamma_+ \text{Tr}[\sigma_+\sigma_+\rho(t)]\} dt_1', \quad (t \geq t'),$$

(20)

$$E[dN_-dN_+] = \{ \gamma_+^2 \text{Tr}[\sigma_+\sigma_+G(t,t')(\sigma_+\rho(t')\sigma_+)] + \delta(t-t')\gamma_+ \text{Tr}[\sigma_+\sigma_+\rho(t)]\} dt_1', \quad (t \geq t'),$$

(21)

$$E[dN_+dN^0_-] = \{ \gamma_+\gamma_\downarrow \text{Tr}[\sigma_+\sigma_+G(t,t')(\sigma_+\rho(t')\sigma_+)]\theta(t-t') + \gamma_\downarrow \gamma_\downarrow \text{Tr}[\sigma_+\sigma_+G(t,t')(\sigma_+\rho(t')\sigma_+)]\theta(t'-t)\} dt_1,$$

(22)

where $t$ ($t'$) is the time of non-vanishing $dN_{\pm}$ ($dN^0_{\pm}$), and doing a careful calculation, we obtain

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

(23)

When we expand the q-number BKE \[11\] accordingly, we find that the coefficients of $\beta$ and $\beta^2$ are indeed the right hand sides of Eqs. (19) and (23). Higher orders of $\beta$ can be checked analogously. But the calculation becomes very long and tedious dramatically.

**Characteristic function of the work.** The preceding argument about the equivalence of Eq. (11) and Eq. (13) is useful. 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 \[13\] as (see the Supplemental Material)

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

(24)

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

$$\begin{cases}
\partial_0 K(t', T; u) = -L^*_t K(t', T; u) - K(t', T; u) \frac{i}{\hbar} [H_1(t'), e^{iuH_0}] e^{-iuH_0}, \\
K(T, T; u) = I.
\end{cases}$$

(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 agrees with the simulation data \[30\] excellently.

**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 shall be related to the quantum Jarzynski equality. This study is underway.
FIG. 1: The ratio of the second and first moments of the quantum work (in unit $\hbar \omega$) with respect to different perturbation strength $\lambda_0$ (in unit $\hbar \omega$) for the TLS model in Ref. [30], where $T \omega/2\pi=10$, $\beta \hbar \omega=2.0$. The crosses ($\gamma_\downarrow=0.02\omega$) and stars ($\gamma_\downarrow=0.01\omega$) are the data of the quantum jump simulation [30], while the open squares and circles are the numerical results of Eqs. (19) and (23). The inset shows the pdf of the quantum work. The dashed bars are from the simulation of Ref. [30], and the solid black bars are obtained by our characteristic function method, where $\beta \hbar \omega=1.0$, $\gamma_\downarrow=0.05\omega$, $\lambda_0=0.05\hbar \omega$.

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[54] Hekking and Pekola should first present the c-number BKE [30]. However, they claimed that they verified the quantum Jarzynski equality. Compared with the method developed in this work, Their method is relatively complex.
[55] These equations are the generalizatoins of Eq. (4.50) in the book of Wiseman and Milburn [36].
I. DERIVATIONS OF EQUATIONS (19) AND (23)

For Eq. (19), the situation is simple:

\[
E[W] = E[\epsilon_n] - E[\epsilon_m] + \hbar \omega E[N_+] - \hbar \omega E[N_-]
\]

\[
= \text{Tr}[H_0 \rho(T)] - \text{Tr}[H_0 \rho(0)] + \int_0^T \text{Tr}[i \hbar \omega (\gamma \sigma_+ \sigma_- - \gamma \sigma_- \sigma_+ \rho(t))] dt_1
\]

\[
= \int_0^T dt_1 \frac{d}{dt_1} \text{Tr}[H_0 \rho(t_1)] - \int_0^T dt_1 \text{Tr}[D^*[H_0] \rho(t_1)]
\]

\[
= \int_0^T dt_1 \text{Tr}[\frac{i}{\hbar}[H_1(t_1), H_0] \rho(t_1)].
\]

(26)

For Eq. (23), however, the proof becomes very tricky. First we write down the original definition of the second moment of the quantum work (13),

\[
E[W^2] = E[\epsilon_n^2 + \epsilon_m^2 - 2\epsilon_n \epsilon_m] + 2\hbar \omega E[\epsilon_n N_+ - \epsilon_n N_- - \epsilon_m N_+ + \epsilon_m N_-] + (\hbar \omega)^2 E[N_+^2 - 2N_+ N_- + N_-^2].
\]

(27)

The first two averages can be rewritten using the density matrix \(\rho(t)\) and the propagator \(G(t_2, t_1)\) as

\[
\text{Tr}[H_0^2 \rho(T)] + \text{Tr}[H_0^2 \rho(0)] - 2 \text{Tr}[H_0 G(T, 0) H_0 \rho(0)]
\]

(28)

and

\[
\int_0^T dt_1 \text{Tr}[\gamma_1 H_0 G(T, t_1) \sigma_- \rho(t_1) \sigma_+] - \int_0^T dt_1 \text{Tr}[\gamma_1 H_0 G(T, t_1) \sigma_+ \rho(t_1) \sigma_-]
\]

\[
- \int_0^T dt_1 \text{Tr}[\gamma_1 \sigma_+ \sigma_- G(t_1, 0) H_0 \rho(0)] + \int_0^T dt_1 \text{Tr}[\gamma_1 \sigma_- \sigma_+ G(t_1, 0) H_0 \rho(0)],
\]

(29)

respectively. For the last average in Eq. (27), we have to resort to Eqs. (20)-(22) and obtain

\[
2 \int_0^T dt_1 \int_0^T dt_2 \text{Tr}[\gamma_2 \sigma_+ \sigma_- G(t_2, t_1) \sigma_- \rho(t_1) \sigma_+] + \int_0^T dt_1 \text{Tr}[\gamma_2 \sigma_+ \sigma_- \rho(t_1)]
\]

\[
- 2 \int_0^T dt_1 \int_0^T dt_2 \text{Tr}[\gamma_1 \sigma_+ \sigma_- G(t_2, t_1) \sigma_+ \rho(t_1) \sigma_-] - \int_0^T dt_1 \int_0^T dt_2 \text{Tr}[\gamma_1 \sigma_+ \sigma_- G(t_2, t_1) \sigma_- \rho(t_1) \sigma_+]
\]

\[
+ 2 \int_0^T dt_1 \int_0^T dt_2 \text{Tr}[\gamma_2 \sigma_- \sigma_+ G(t_2, t_1) \sigma_+ \rho(t_1) \sigma_-] + \int_0^T dt_1 \text{Tr}[\gamma_2 \sigma_- \sigma_+ \rho(t_1)].
\]

(30)

Substituting Eqs. (28)-(30) into Eq. (27) and doing a rearrangement, we have

\[
E[W^2] = 2(\hbar \omega)^2 \int_0^T dt_1 \int_0^T dt_2 \text{Tr}[(\gamma_1 \sigma_+ \sigma_- - \gamma_1 \sigma_- \sigma_+) G(t_2, t_1) (\gamma_1 \sigma_- \rho(t_1) \sigma_+ - \gamma_1 \sigma_+ \rho(t_1) \sigma_-)]
\]

\[
+ 2\hbar \omega \int_0^T dt_1 \text{Tr}[H_0 G(T, t_1) (\gamma_1 \sigma_- \rho(t_1) \sigma_+ - \gamma_1 \sigma_+ \rho(t_1) \sigma_-)]
\]

\[
- 2\hbar \omega \int_0^T dt_1 \text{Tr}[(\gamma_1 \sigma_+ \sigma_- - \gamma_1 \sigma_- \sigma_+) G(t_1, 0) H_0 \rho(0)]
\]

\[
+ \text{Tr}[H_0^2 \rho(T)] + \text{Tr}[H_0^2 \rho(0)] - 2 \text{Tr}[H_0 G(T, 0) H_0 \rho(0)]
\]

\[
+ (\hbar \omega)^2 \int_0^T dt_1 \text{Tr}[\gamma_1 \sigma_+ \sigma_- \rho(t_1)] + (\hbar \omega)^2 \int_0^T dt_1 \text{Tr}[\gamma_1 \sigma_- \sigma_+ \rho(t_1)].
\]

(31)

At this step, we do not see that Eq. (31) essentially equals to the right hand side of Eq. (23). In order to go head, we need to introduce two additional equations:

\[
L_1[H_0 \rho] = H_0 L_1[\rho] - \frac{i}{\hbar}[H_1(t), H_0] \rho + \hbar \omega (\gamma \sigma_+ \rho \sigma_+ - \gamma \sigma_- \rho \sigma_-),
\]

(32)

\[
L_1^*[H_0 H_0] = \frac{i}{\hbar}[H_1(t), H_0] H_0 + \frac{i}{\hbar}[H_0 [H_1(t), H_0] + 2D^*[H_0] H_0 + (\hbar \omega)^2 \gamma \sigma_+ \sigma_- + (\hbar \omega)^2 \gamma \sigma_- \sigma_+.
\]

(33)
Using the expression of $D^*[H_0]$ in Eq. (20), the definition of the adjoint propagator $G^*(t_1, t_2)$, the above two equations, and carrying out further calculations we obtain

$$\frac{1}{2}E[W^2] = -\int_0^T dt_1 \int_0^T dt_2 \text{Tr}[D^*[H_0]G(t_2, t_1)\frac{i}{\hbar}[H_1(t_1), H_0]\rho(t_1)]$$

$$+ \int_0^T dt_1 \text{Tr}[H_0 G(T, t_1)\frac{i}{\hbar}[H_1(t_1), H_0]\rho(t_1)]$$

$$- \frac{1}{2}\int_0^T dt_1 \text{Tr}\left[\frac{i}{\hbar}[H_1(t_1), H_0]\rho(t_1)\right] - \frac{1}{2}\int_0^T dt_1 \text{Tr}\left[H_0 \frac{i}{\hbar}[H_1(t_1), H_0]\rho(t_1)\right].$$

(34)

Using the property of $G^*(t_1, t_2)$,

$$\partial_{t_2}[G^*(t_1, t_2)H_0] = G^*(t_1, t_2)\frac{i}{\hbar}[H_1(t_1), H_0] + G^*(t_1, t_2)D^*[H_0],$$

(35)

we finally arrive at the right hand side of Eq. (23). Noting that $G^*(t_1, t_2)$ is a superoperator that acts on the operator on its right hand side.

II. CALCULATING $K(t', T; u)$ FOR THE TSL MODEL

For the simple resonant TSL model in Ref. [30], we may write the operator $K(t', T; u)$ in the Pauli matrices as

$$K(t', T; u) = \frac{1}{2}[k_0(t')I + k_x(t')\sigma_x + k_y(t')\sigma_y + k_z(t')\sigma_z].$$

(36)

Substituting it into Eq. (25) and doing a simple derivation, we obtain

$$k_0^\prime = \frac{i}{2}e^{-iu}(e^{iu} - 1)^2\lambda(t')k_x - \frac{1}{2}e^{-iu}(e^{2iu} - 1)\lambda(t')k_y + (\gamma_+ - \gamma_\uparrow)k_z,$$

(37)

$$k_x^\prime = \frac{i}{2}e^{-iu}(e^{iu} - 1)^2\lambda(t')k_0 + \frac{1}{2}(\gamma_+ + \gamma_\uparrow)k_x - \omega k_y + \frac{i}{2}e^{-iu}(e^{2iu} - 1)\lambda(t')k_z,$$

(38)

$$k_y^\prime = \frac{1}{2}e^{-iu}(1 - e^{2iu})\lambda(t')k_0 + \omega k_x + \frac{1}{2}(\gamma_+ + \gamma_\uparrow)k_y - \frac{1}{2}e^{-iu}(1 + e^{iu})^2\lambda(t')k_z,$$

(39)

$$k_z^\prime = \frac{i}{2}e^{-iu}(1 - e^{2iu})\lambda(t')k_x + \frac{1}{2}e^{-iu}(1 + e^{iu})^2\lambda(t')k_0 + (\gamma_+ + \gamma_\uparrow)k_z,$$

(40)

where the dots denote the time derivative $d/dt'$, $\lambda(t')=\lambda_0\omega\sin(\omega t')$, and the terminal conditions are $k_0(T)=2$, $k_x(T)=k_y(T)=k_z(T)=0$, respectively. The reader is reminded that all parameters are dimensionless. We clearly see that the operator $K$ is periodic with respect to $u$, i.e. $K(t', T; u + 2n\pi)=K(t', T; u)$ for arbitrary integer $n$. This feature ensures that the pdf of the quantum work is discrete after we perform the inverse Fourier transform for $\Phi(u)$. These differential equations can be easily solved numerically as a terminal problem, e.g., by using the Mathematica.

III. GENERAL QMMEs HAVING STRUCTURE OF EQ. (1)

We have mentioned that Eq. (1) is a simplest example of the specific type of QMMEs. The dissipation parts of these QMMEs have the following common structure

$$D[\rho] = \sum_j \gamma_j^\uparrow(A^\dagger_j \rho A^\downarrow_j - \frac{1}{2}\{\rho, A^\dagger_j A^\downarrow_j\}) + \gamma_j^\downarrow(\rho A^\dagger_j A^\downarrow_j - \frac{1}{2}\{\rho, A^\dagger_j A^\downarrow_j\}),$$

(41)

where the Lindblad operators are the eigenoperators of the free Hamiltonian $H_0$, i.e., $[H_0, A^\dagger_j]=\pm\hbar\omega_j A^\downarrow_j$, and the damping rates are assumed to satisfy $\gamma_j^\dagger=\gamma_j^\uparrow \exp(-\beta\hbar\omega_j)$. Except for the additional summation over all possible coupling channels $j$ of the system with the heat bath, we do not see that there are fundamental differences between the generalized and the simplest QMMEs. Therefore, all general results in the main text could be simply extended
into the general situation by changing $\sigma_\pm \rightarrow A_\pm^1$, $N_\pm \rightarrow N_\pm^1$, $\omega \rightarrow \omega_i$, $\gamma_\uparrow \rightarrow \gamma_i^\uparrow$, and doing appropriate summation over the various channels $j$, e.g., the quantum work for the QMMEs with Eq. (41) is

$$W = \epsilon_n - \epsilon_m + \sum_j \hbar \omega_j N_j^+ - \sum_j \hbar \omega_j N_j^-.$$  \hspace{1cm} (42)

Noting that the three Eqs. (20)-(22) are not zero only for the same channels.