Calculating work in adiabatic two-level quantum Markovian master equations: characteristic function method

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We present a characteristic function method to calculate the probability density functions of the inclusive work in the adiabatic two-level quantum Markovian master equations. These systems are slowly steered by some external parameters and the dissipations may depend on time. The foundation of the theory is the interpretation of the quantum jump on the master equations. In addition to the applications of calculation, we also find that the characteristic functions can account for the fluctuation characteristics of the work from the symmetry of these functions. This fully agrees with the case in the isolated systems. A concrete two-level model is used to show our method.

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I. INTRODUCTION

In the past decade, extending classical work equalities\cite{1,2} into the nonequilibrium quantum regime has attracted intensive interest\cite{2, 4, 6}. With the growing consensus about the definitions of the quantum work and their equalities in isolated quantum Hamiltonian systems\cite{8, 10, 12, 14, 16, 19, 20, 21, 22, 23, 25, 26}, recently, some attentions were devoted to the quantum Markovian master equations (QMMEs)\cite{9, 10, 12, 14, 16, 19, 20, 21, 22, 23, 25, 26}. For instance, on the basis of the two energy measurement scheme\cite{20} and the quantum jump theory\cite{30, 32}, Horowitz\cite{22} proved a quantum Jarzynski equality (QJE) for a specific type of master equations. These equations are assumed to have instantaneous thermal equilibrium solutions. With a similar idea, Hekking and Pekola\cite{25} numerically verified the JE in a concrete quantum two-level system (TLS). This system is driven by a weak external field and the dissipation is time-independent. Hence, the assumption of Ref.\cite{22} is not held in this case. Their result was clarified soon by us to be the quantum counterpart of the Bochkov-Kuzovlev equality (BKE)\cite{1} instead of the JE\cite{20}. On the other hand, Chetrite and Mallick\cite{23} proposed an alternative QJE in the master equations that have instantaneous steady-state solutions. However, different from the mentioned studies, their equality is an abstract “book-keeping” of a sum of multiple time correlation functions of operators. Interestingly, the scheme of the energy measurement and the notion of the quantum jump were not exploited by the authors.

Although these achievements are significant\cite{1, 11, 12, 16, 22, 23, 25, 26}, we notice that most of them focused on the formal derivations of the work equalities in various QMMEs. Few\cite{23, 26} have genuinely calculated the probability density functions (pdfs) of the quantum work in concrete models. In our opinion the current situation is still not very satisfactory. After all, the pdf of the work is fundamental. The equality that it satisfies is held only under the specific conditions\cite{12, 23}. Moreover, previous results shown that effectively calculating the pdf is usually very challenging even in the isolated systems\cite{24}. Hence, the calculation of the pdf of the quantum work in the master equations deserves serious investigation, which is main motivation of this paper.

As one of statistical interpretations of the QMMEs with the Lindblad form\cite{34, 36}, the quantum jump theory\cite{30–32} also provides promising definitions of the quantum work\cite{10, 13, 16, 22, 23, 25, 27, 29}. By repeatedly simulating quantum trajectories while recording the quantum jumps, one may readily construct the statistic histogram about the work\cite{23}. Although this method is straightforward, it is inconvenient in theoretical investigations. For instance, the simulation cannot tell us how the moments of the work are related to the master equations. In addition, the simulation has to be faced the errors of statistical sampling. Very recently, in a specific type of master equations an alternative method was developed\cite{26}. It is based on solving the characteristic function (CF) of the exclusive quantum work\cite{37}. In addition to obtaining the closed expressions of the moments of the work, we found that its numerical implement was also simple. Due to these attractive features, here we try to extend the previous CF method to the case of the inclusive quantum work\cite{37} in the adiabatic master equation\cite{38, 42}. These equations describe the dynamics of the dissipated systems that are adiabatically steered by some external parameters. They were often utilized to model the decoherence effect of thermal environment in the adiabatic quantum computations\cite{43–47}.

The paper is organized as follows. In Sec. II we review a generic two-level adiabatic QMME and its interpretation from the point of view of the quantum jump. The essential notations are set up. In Sec. III we define the backward equation of the forward master equation. In Sec. IV we prove that the QJE in the same forward equation possesses two different expressions. On the basis of this finding, in Sec. V we present the CF method to calculate the pdf of the inclusive quantum work. In Sec. VI a concrete TLS model is used to verify our theory. Section VII is the conclusion of the paper.

II. TWO-LEVEL ADIABATIC QMME AND QUANTUM JUMP INTERPRETATION

For simplicity in notations, throughout this paper we employ a generic two-level adiabatic QMME to develop our theory. The most general form of the equation can be found in Ref.\cite{40}. Although we will use the Pauli matrices, we do not consider the degrees of freedom of spin here. In time interval \((0, t_f)\) the TLS evolves under an adiabatically varying Hamiltonian \(H(t)\). Meanwhile, the system exchanges energy with the heat bath at inverse temperature \(\beta\). We assume the interaction Hamiltonian of the system and the heat bath to be \(H_I = A \otimes B\). Under the weak-coupling Markovian approximation, the secular approximations, and the adiabatic condition, the equation of motion of the reduced density matrix \(\rho(t)\) of the system has been established\cite{38, 42}.

\[
\partial_t \rho(t) = \mathcal{L}_I \rho(t) = -\frac{i}{\hbar} [H(t), \rho(t)] + D_I [\rho(t)].
\]

The time-dependent dissipation term is

\[
D_I [\rho] = \sum_{\alpha = \pm} \gamma_\alpha(\omega_\alpha) \left[ A_\alpha(t) \rho A_\alpha^\dagger(t) - \frac{1}{2} \{ A_\alpha^\dagger(t), A_\alpha(t), \rho \} \right] + \gamma_0 \left[ A_0(t) \rho A_0^\dagger(t) - \frac{1}{2} \{ A_0^\dagger(t), A_0(t), \rho \} \right].
\]
The rates $\gamma_{\pm}(\omega)$ and $\gamma_0$ equal $\Gamma(\mp \omega)$ and $\Gamma(0)$, respectively, where $\Gamma(\omega) = \int_{-\infty}^{\infty} d\varepsilon e^{i\varepsilon \tau} \langle B(\tau) B(0) \rangle_{eq}$ and the average is associated with the thermally equilibrium heat bath. The Lindblad operators $A_{\pm}(t)$ and $A_0(t)$ are

$$|\varepsilon_+(t)\rangle\langle\varepsilon_+(t)|A_\pm(t)|\varepsilon_+(t)\rangle,$$

and

$$\sum_{\alpha=\pm} |\varepsilon_\alpha(t)\rangle\langle\varepsilon_\alpha(t)| A|\varepsilon_\alpha(t)\rangle,$$

respectively, where $|\varepsilon_\pm(t)\rangle$ are the adiabatic (instantaneous) eigenvectors of the Hamiltonian $H(t)$ with eigenvalues $\varepsilon_\pm(t)$. These operators have properties as $A_{\pm}^\dagger(t) = A_{\mp}(t)$, $A_0^\dagger(t) = A_0(t)$,

$$[H(t), A_{\pm}(t)] = \pm i \hbar \omega_\mp A_{\pm}(t),$$

and $[H(t), A_0(t)] = 0$, where $\hbar \omega_\pm = \varepsilon_+(t) - \varepsilon_-(t)$. The crucial assumption on which this paper depends is the instantaneous detailed balance condition, $\gamma_+(\omega_i) = \gamma_-(\omega_i)e^{-\beta\hbar\omega_i}$. In addition, we also specify that the correlation function of the heat bath has an Ohmic spectral density $\frac{\beta}{2\pi} \omega$, namely, $\gamma_0 = \kappa / \beta \hbar$ and $\gamma_-(\omega) = \kappa \omega / (1 - e^{-\beta \hbar \omega})$, where $\kappa$ is the coupling strength. The structure of the adiabatic master equation (1) and the instantaneous detailed balance condition imply that the TLS always has instantaneous thermal state

$$\rho_{eq}(t) = \frac{e^{-\beta\varepsilon_\alpha(t)}}{Z(t)} |\varepsilon_\alpha(t)\rangle\langle\varepsilon_\alpha(t)| = \sum_{\alpha=\pm} \rho_{eq}^\alpha(t)|\varepsilon_\alpha(t)\rangle\langle\varepsilon_\alpha(t)|,$$

where $Z(t) = Tr[e^{-\beta H(t)}]$ is the instantaneous partition function at time $t$. Finally, we set the initial density matrix to be $\rho_{eq}(0)$ unless other explicitly stated. The conditions of the physical validity of Eq. (1) have been discussed in details [40, 42].

According to the quantum jump theory [30-32], the density matrix $\rho(t)$ can be regarded as a statistical average of the wave function $\psi(t)$. This wave function varies in the Hilbert space of the TLS by alternatively deterministic continuous evolution and stochastic jumps. Its deterministic equation of motion is

$$\partial_t \psi(t) = -\frac{i}{\hbar} H(t) \psi(t)$$

$$= -\frac{i}{\hbar} H(t) \psi(t) - \frac{1}{2} \left( \sum_{\alpha=\pm} \gamma_\alpha(\omega_i) A_{\alpha}^\dagger(t) A_\alpha(t) + \gamma_0 A_0^\dagger(t) A_0(t) \right) \psi(t).$$

Occasionally, the continuous evolution is interrupted by a jump to one of the three states: $A_{\pm}(t)\psi(t)/\|A_{\pm}(t)\psi(t)\|$ and $A_0(t)\psi(t)/\|A_0(t)\psi(t)\|$. We name them $A_\pm$- and $A_0$-jumps, respectively. The probabilities of these jumps are proportional to $\gamma_\pm(\omega_i)\|A_{\pm}(t)\psi(t)\|^2$ and $\gamma_0\|A_0(t)\psi(t)\|^2$, respectively. For the simple TLS the wave function $\psi(t)$ can be always written as $\sum_{\alpha=\pm} \varepsilon_\alpha(t)|\varepsilon_\alpha(t)\rangle$. Hence, after jump the former two states are indeed $|\varepsilon_\pm(t)\rangle$, while their jumping probabilities are proportional to $\gamma_\pm(\omega_i)|\varepsilon_\pm(t)\rangle|^2$. We see that the latter is physically intuitive. From the energetic point of view, $A_\pm$-jumps accompany an absorption and a release of one energy $\hbar \omega_\pm$ from the system and to the heat bath, respectively. On the contrary, the $A_0$-jump only induces the changes of the local phases of the wave function [30-32]. Given the above explanations, the probability of observing a trajectory in the time interval $(0, t)$ that its initial state is $|\psi_0\rangle$, undergoes $N$ jumps at increasing times $t_i$ ($i=1, \cdots, N$) with an order of jumps $(A_{\alpha_1}, \cdots, A_{\alpha_N})$ is

$$\prod_{i=1}^{N} dt_i \prod_{i=1}^{N} \gamma_{\alpha_i} \|L_N(t, 0)|\psi_0\rangle\|^2$$

$$= \prod_{i=1}^{N} dt_i \prod_{i=1}^{N} \gamma_{\alpha_i} \|U(t, t_N) A_{\alpha_1}(t_N) \cdots U(t_2, t_1) A_{\alpha_1}(t_1) U(t_1, 0)|\psi_0\rangle\|^2.$$

Here $\alpha_i$ equals $\pm$ or $0$, and we did not explicitly write out $\omega_i$ in $\gamma_{\pm}$. Additionally, the notation $U$ is the non-unitary time evolution operator of Eq. (7) in a certain time interval, e.g., $U(t_2, t_1) = T_{\tau} \exp[-\frac{i}{\hbar} \int_{t_1}^{t_2} d\tau \hat{H}(\tau)]$. Here $T_{\tau}$ denotes the chronological time-ordering operator. With the probability density of the quantum trajectory and doing a summation over all trajectories, one can calculate the density matrix by the wave-function according to $\rho(t) = E[|\psi(t)\rangle\langle\psi(t)|]$ [31].
III. BACKWARD ADIABATIC QMMES

The work equalities are intimately related to the symmetric properties of the system and its time-reversal \[13, 32\]. As a preliminary of the following discussion, we introduce the time-reversal of the forward Eq. (11), or the backward adiabatic QMME. First we define $\hat{H}(s) = \Theta H(t)\Theta^\dagger$ as the time-reversed Hamiltonian, where $\Theta$ is the time-reversal operator. We also introduced the other time parameter $s = t_f - t$. Throughout this paper, we use the notations with \textit{tilde} to denote their meanings under the time-reversal. Obviously, the eigenvalues $\tilde{\varepsilon}_\alpha(s)$ of $\hat{H}(s)$ equal $\Theta |\varepsilon_\alpha(t)|$ and $\varepsilon_\alpha(t)$, respectively. If the interaction Hamiltonian $H_I$ is time reversible, which we only consider here, we may establish the backward quantum master equation as

$$
\partial_s \tilde{\rho}(s) = \tilde{L}_s \tilde{\rho}(s) = -\frac{i}{\hbar} \left[ \hat{H}(s), \tilde{\rho}(s) \right] + \tilde{D}_s [\tilde{\rho}(s)]. \tag{9}
$$

The dissipation term is

$$
\tilde{D}_s[\tilde{\rho}] = \sum_{\alpha=\pm} \gamma_{\alpha}(\tilde{\omega}_s) \left[ A_{\alpha}(s)\tilde{\rho}\tilde{A}_{\alpha}^\dagger(s) - \frac{1}{2} \left\{ \tilde{A}_{\alpha}^\dagger(s)\tilde{A}_{\alpha}(s), \tilde{\rho} \right\} \right] + \gamma_0 \left[ \tilde{A}_0(s)\tilde{\rho}\tilde{A}_0^\dagger(s) - \frac{1}{2} \left\{ \tilde{A}_0^\dagger(s)\tilde{A}_0(s), \tilde{\rho} \right\} \right]. \tag{10}
$$

The time-reversed rates and Lindblad operators have simple connections with the original ones: $\tilde{\gamma}_{\alpha}(\tilde{\omega}_s) = \gamma_{\alpha}(\omega_t)$, $\gamma_0 = \gamma_0$, $\tilde{A}_{\pm}(s) = \Theta A_{\pm}(t)\Theta^\dagger$ and $\tilde{A}_0(s) = \Theta A_0(t)\Theta^\dagger$. Compared Eq. (11) with (1), we see that the former may be simply obtained from the latter by replacing $t$ by $s$ and adding tildes on all relevant quantities therein. Because the backward equation is still adiabatic, it has the interpretation of the quantum jump as well. For instance, the deterministic evolution equation for Eq. (11) is,

$$
\partial_s \tilde{\psi}(s) = -\frac{i}{\hbar} \hat{\tilde{H}}(s)\tilde{\psi}(s), \tag{11}
$$

where $\hat{\tilde{H}}(s)$ is analogous to $\hat{H}(t)$ in Eq. (1) except that the operators and rates therein are replaced by their time-reversals.

IV. TWO EXPRESSIONS OF QJE

In order to establish the CF method about the inclusive quantum work, we first prove the equivalence of two expressions of QJE in the same adiabatic master equation \[1\]. These QJEs were respectively proposed by Horowitz \[22\] and Chetrite and Mallick \[23\] using very different theories and techniques. Following our previous convention \[26\], we name them the \textit{c-} and \textit{q-number} QJEs, respectively. So far their relation was not clarified. The reader will see that this equivalent demonstration indeed provides a simple way toward an important evolution equation that assists the calculation of the CF.

A. \textit{c-number QJE}

Let us choose an arbitrary time $t'$ between 0 and $t_f$ and suppose that the wave function at the time is $|\varepsilon_\alpha(t')\rangle$. Given a quantum trajectory of Eq. (11) starting with this state. If we record the order of jumps $(A_{\alpha_1}, \cdots, A_{\alpha_N})$ at later times $(t_1, \cdots, t_N)$, and measure the energy eigenvector of the TLS at the terminal time $t_f$ to be $|\varepsilon_\delta(t_f)\rangle$, we define the inclusive quantum work done on the system along the trajectory in the time interval $(t', t_f)$ as

$$
W(t') = \varepsilon_\delta(t_f) - \varepsilon_\alpha(t') - \int_{t'}^{t_f} \hbar \omega_\tau dN_+(\tau) + \int_{t'}^{t_f} \hbar \omega_\tau dN_-(\tau), \tag{12}
$$

where $dN_\pm(\tau)$ represent the increments of the $A_\pm$-jumps at instantaneous time $\tau$. Note that the number $N_0$ of the $A_0$-jump is not involved since these jumps do not contribute any energy changes. Under these notations, now we are concerned about the following equation,

$$
e^{-\beta W(t')} \prod_{i=N}^1 d\gamma_i \prod_{i=N}^1 \gamma_i |\langle \varepsilon_\delta(t_f)|L_N(t_f, t')|\varepsilon_\alpha(t')\rangle|^2 \tilde{p}_\alpha^{eq}(t'), \tag{13}
$$

where $N$ is the total number of the three jumps. According to Eq. (8), the whole term in the square brackets is the conditional probability of observing the trajectory. Hence, its product with $p_\alpha^{eq}(t')$ is the joint probability.
Equation (13) possesses an intriguing explanation of time reversal [16, 22]. We first notice that the terms in the exponential function of the work can be combined into the rates using the instantaneous detailed balance condition. Then we rewrite the equation as

$$Z(t_f) Z(t') \left[ \prod_{i=1}^{N} \gamma_{\tilde{\alpha}_i} ||\langle \varepsilon_{\alpha_i}(t')|\Theta \tilde{\mathcal{L}}_N(s',0)\Theta |\varepsilon_{\delta}(t_f)\rangle||^2 \right] p^\varepsilon_{\delta}(t_f), \quad (14)$$

where $\tilde{\alpha}_i$ denotes $\mp$ or 0 if $\alpha_i$ is $\pm$ or 0, respectively. The operator $\tilde{\mathcal{L}}_N(s',0)$ with $t' + s' = t_f$ is

$$[\Theta U^\dagger(t_1,t')\Theta^\dagger][\Theta A^\dagger_{\alpha_1}(t_1)\Theta^\dagger] \cdots [\Theta U^\dagger(t_N,t_{N-1})\Theta^\dagger][\Theta A^\dagger_{\alpha_N}(t_N)\Theta^\dagger][\Theta U^\dagger(t_f,t_N)\Theta^\dagger]. \quad (15)$$

We immediately see that the term in the second square brackets is just $\tilde{A}_{\tilde{\alpha}_N}(s_N)$ of the backward adiabatic QMME. Here we define $s_j + t_i = t_f$ and $i + j = N + 1$. Note that the jumps of $\tilde{A}_{\tilde{\alpha}_i}$ and $A_{\alpha_i}$ are opposite unless $\alpha_1 = 0$. Moreover, we may check that the term in the first square brackets is the non-unitary time evolution operator $\tilde{U}(s', s_N)$ of Eq. (11) in the time interval $(s_N, s')$. For the remaining terms in the same equation these two observations are as well true. Noting $\tilde{\gamma}_{\tilde{\alpha}_i}(\tilde{\omega}_{s_i}) = \gamma_{\tilde{\alpha}_i}(\omega_{s_i})$, we finally find that the whole term in the square brackets in Eq. (14) is nothing but the conditional probability of a quantum trajectory for the backward master equation: its state at time 0 is $\Theta |\varepsilon_{\delta}(t_f)\rangle$, the order of jumps is $(\tilde{A}_{\tilde{\alpha}_N}, \cdots, \tilde{A}_{\tilde{\alpha}_1})$ at times $(s_1, \cdots, s_N)$, and the energy eigenvector measured at the final time $s'$ is $\Theta |\varepsilon_{\alpha}(t')\rangle$. Fig. (1) is a schematic diagram of two time-revered quantum trajectories.

We now do a summation of Eq. (13) over all quantum trajectories that start with the same $|\varepsilon_{\alpha}(t')\rangle$ and end at all
the energy eigenvectors. Using Eq. (13) we establish an important relation

$$E_{\alpha}[e^{-\beta W(t')}|\tilde{\rho}_{eq}^{s'}(t') = \frac{Z(t_f)}{Z(t')} \langle \varepsilon_{\alpha}(t')|\Theta^\dagger \tilde{\rho}(s')\Theta|\varepsilon_{\alpha}(t')\rangle.]$$ \hspace{1cm} (16)$$

We used $E_{\alpha}$ to denote that all trajectories start with the same quantum state. The reduced density matrix $\tilde{\rho}(s')$ is the solution of Eq. (9) at time $s'$. Particularly, its initial condition $\tilde{\rho}(0)$ has been specified at the thermal state $\Theta \rho_{eq}(t_f)\Theta^\dagger$. If we further sum Eq. (16) over the index $\alpha$ and choose $t' = 0$, we obtain the $c$-number QJE in the two-level adiabatic master equation (1):

$$E[e^{-\beta W}] = e^{-\beta \Delta G},$$ \hspace{1cm} (17)$$

where $\beta \Delta G = \ln Z(t_f) - \ln Z(0)$, and we used a notation $W$ for $W(0)$. The reader is reminded that in this case the initial condition of the forward Eq. (11) must be the thermal state. This explain why we set up this condition at the beginning.

**B. $q$-number QJE**

Equation (16) implies that it may arise from an almost trivial operator identity:

$$R(t', t_f)\rho_{eq}(t') = \Theta^\dagger \tilde{\rho}(s')\Theta.$$ \hspace{1cm} (18)$$

Note that its validity has nothing to do with the quantum jump provided the well-defined $\tilde{\rho}(s')$ and $\rho_{eq}(t')$. Writing Eq. (18) in the energy representation, we have an important result

$$\langle \varepsilon_{\alpha}(t')|R(t', t_f)|\varepsilon_{\alpha}(t')\rangle = \frac{Z(t_f)}{Z(t')} E_{\alpha}[e^{-\beta W(t')}].$$ \hspace{1cm} (19)$$

Obviously, the operator $R(t', t_f)$ possesses all characteristics that the $E_{\alpha}$-term has. In the following we discuss the general properties of $R(t', t_f)$ and temporarily set aside the quantum jump theory. Substituting Eq. (18) into Eq. (9), we can obtain the evolution equation of $R(t', t_f)$ with respect to $t'$

$$\partial_{t'} R(t', t_f) = -\mathcal{L}_{t'} R(t', t_f) - R(t', t_f)\partial_{t'} \rho_{eq}(t')\tilde{\rho}_{eq}^{-1}(t'),$$ \hspace{1cm} (20)$$

where the adjoint superoperator of $\mathcal{L}_{t'}$ is

$$\mathcal{L}_{t'}^\dagger O = \frac{i}{\hbar} \{H(t'), O\} + \sum_{\alpha = \pm} \gamma_{\alpha}(\omega) \left[ A_{\alpha}^\dagger(t') O A_{\alpha}(t') - \frac{1}{2} \{ A_{\alpha}^\dagger(t') A_{\alpha}(t'), O \} \right] + \gamma_0 \left[ A_{0}^\dagger(t') O A_{0}(t') - \frac{1}{2} \{ A_{0}^\dagger(t') A_{0}(t'), O \} \right].$$ \hspace{1cm} (21)$$

To arrive at Eq. (20), we have applied the instantaneous detailed balance condition. Here we must emphasize that the derivation does not matter with what the initial conditions of the forward and backward master equations are. Equation (20) is a terminal value problem, i.e., $R(t_f, t_f) = I$ the identity operator. Introducing the adjoint propagator $G^*(t_1, t_2) = T_+ \exp[\int_{t_1}^{t_2} dt \mathcal{L}_{t'}^\dagger]$ (22), where $T_+$ denotes the antichronological time-ordering operator, we may obtain a formal solution of Eq. (20) written as the celebrated Dyson series \cite{23, 26, 50}. Choosing $t' = 0$ and taking traces of two sides of Eq. (18), we obtain the $q$-number QJE \cite{23, 50} for the same adiabatic master equation (1):

$$\langle T_+ \exp \left[ \int_0^{t_f} d\tau W(\tau) \right] \rangle = e^{-\beta \Delta G}.$$ \hspace{1cm} (22)$$

Here we have defined an operator $W(\tau) = \partial_{\tau} e^{-\beta H(\tau)} e^{\beta H(\tau)}$. It is worthy to point out that the “average” notation $\langle \cdots \rangle$ above is a only shorthand \cite{23}. Indeed, its explicit expression is a sum of infinite terms of multiple times correlation functions of operators \cite{31}:

$$1 + \left\langle \int_0^{t_f} dt_1 W(t_1) \right\rangle + \left\langle \int_0^{t_f} dt_1 \int_0^{t_f} dt_2 W(t_2) W(t_1) \right\rangle + \cdots$$

$$= 1 + \int_0^{t_f} dt_1 \text{Tr} [W(t_1) G(t_1, 0) \rho_{eq}(0)] + \int_0^{t_f} dt_1 \int_0^{t_f} dt_2 \text{Tr} [W(t_2) G(t_2, t_1) W(t_1) G(t_1, 0) \rho_{eq}(0)] + \cdots,$$ \hspace{1cm} (23)$$

\[\int_0^{t_f} dt W(t) = \sum_{\alpha = \pm} \gamma_{\alpha}(\omega) \left[ A_{\alpha}^\dagger(t) O A_{\alpha}(t) - \frac{1}{2} \{ A_{\alpha}^\dagger(t) A_{\alpha}(t), O \} \right] + \gamma_0 \left[ A_{0}^\dagger(t) O A_{0}(t) - \frac{1}{2} \{ A_{0}^\dagger(t) A_{0}(t), O \} \right].\]
where \( G(t_2, t_1) = \mathcal{T}_- \exp \left[ \int_{t_1}^{t_2} dt \mathcal{L}_+ \right] \) is the propagator of Eq. (11) [31]. Note that these propagators are superoperators; they act on all terms on their right-hand side.

Equation (19) ensures the equivalence of the \( c- \) and \( q- \) number QJE. An alternative straightforward proof is to expand the exponential functions of Eqs. (17) and (22) as a series of the inverse temperature \( \beta \) and to check whether their coefficients are the same. To implement this scheme, one has to know the correlation functions of the quantum jumps at different times. Fortunately, they have been given by the quantum jump theory [32]. Here we list the final results of the first two coefficients that are in fact the first two moments of the inclusive quantum work:

\[
E[W] = \left\langle \int_0^{t_f} dt_1 \partial_1 H(t_1) \right\rangle, \tag{24}
\]

\[
E[W^2] = 2 \left\langle \int_0^{t_f} dt_1 \int_1^{t_f} dt_2 \partial_1 \partial_2 H(t_2) \partial_1 H(t_1) \right\rangle + \left\langle \int_0^{t_f} dt_1 [H(t_1), \partial_1 H(t_1)] \right\rangle. \tag{25}
\]

Note that the second term in the second equation is a pure quantum effect. We leave the concrete derivations in the Appendix I.

V. CHARACTERISTIC FUNCTION OF QUANTUM WORK

In the preceding discussion about the \( c- \) number QJE, we clearly see that the pdf of the inclusive work [12] can be constructed using the quantum jump simulation [31, 32]. On the contrary, we do not get such an impression in the discussion of the \( q- \) number version. For the latter, a possible way is to calculate all the moments of the work using the equations like Eqs. (24) and (25) and then to convert them into the pdf. Due to the high-dimensional integrations involved and increasing complex of the connections between the moments and the multiple time correlation functions of operators, this scheme is almost infeasible in practice.

To bypass this difficulty, we introduce the CF of the pdf,

\[
\Phi(\mu) = E[e^{i\mu W}], \tag{26}
\]

where \( \mu \) is real number. After solving the CF, the pdf of the inclusive work is obtained by performing an inverse Fourier transform of \( \Phi(\mu) \). At the first glance, Eq. (26) does not show obvious advantages. However, the CF may be simply regarded as the left-hand side of QJE (17) except \( \beta \) replaced by an imaginary inverse temperature \( -i\beta \). Inspired by Eq. (19), we want to find an operator \( K(t', t_f; \mu) \) analogous to \( R(t', t_f) \) by which the CF (26) is calculated according to

\[
\Phi(\mu) = \text{Tr}[K(0, t_f; \mu) \rho_{eq}(0)] = \langle K(0, t_f; \mu) \rangle. \tag{27}
\]

It is not difficult to see that the operator indeed exists if it satisfies an evolution equation

\[
\partial_\mu K(t', t_f; \mu) = -\mathcal{L}_+^* K(t', t_f; \mu) - K(t', t_f; \mu) \partial_\mu e^{i\mu H(t')} e^{-i\mu H(t')}. \tag{28}
\]

The terminal condition is \( K(t_f, t_f; \mu) = I \).

At this stage we have realized our aim of calculating the pdf of the work by solving the differential equation (28) rather than simulating the quantum trajectories. In practice, however, it is inconvenient to compute the exponential functions of the Hamiltonian; see the last term in Eq. (28). Additionally, the above equation is a terminal value problem rather than the conventional initial value problem. These two undesirable features can be remedied by introducing another operator

\[
\tilde{K}(s'; \mu) = \Theta K(t', t_f; \mu) e^{i\mu H(t')} \Theta^\dagger. \tag{29}
\]

After a simple algebra we have

\[
\partial_\mu \tilde{K}(s'; \mu) = \tilde{\mathcal{L}}_+ \tilde{K}(s'; \mu), \tag{30}
\]

and the initial condition \( \tilde{K}(0; \mu) \) equals \( e^{-i\mu \tilde{H}(0)} \). The superoperator of the right-hand side of Eq. (30) is

\[
\tilde{\mathcal{L}}_+(\mu) O = -\frac{i}{\hbar} \tilde{H}(s), O] + \sum_{\alpha = \pm} \tilde{\gamma}_\alpha (\tilde{\omega}_s) [e^{i\alpha \hbar \tilde{\omega}_s} \tilde{A}_\alpha^I(s) O \tilde{A}_{\alpha}(s) - \frac{1}{2} \{ \tilde{A}_\alpha^I(s) \tilde{A}_\alpha^I(s), O \}
\]

\[
+ \tilde{\gamma}_0 [\tilde{A}_0^I(s) O \tilde{A}_0(s) - \frac{1}{2} \{ \tilde{A}_0^I(s) \tilde{A}_0^I(s), O \}]. \tag{31}
\]
Accordingly, Eq. (27) is also slightly modified as

\[
\Phi(\mu) = \frac{1}{Z(0)} \text{Tr}[\Theta^\dagger \overline{\mathcal{K}}(t_f; \mu) \Theta e^{i(\mu + \beta) H(0)}] \\
= \frac{1}{Z(0)} \text{Tr}[\overline{\mathcal{K}}(t_f; -\mu) e^{i(\mu + \beta) H(0)}].
\] (32)

The second equation is due to \( \text{Tr}[\Theta^\dagger O \Theta] = \text{Tr}[O^\dagger] \). We see that Eq. (31) is very close to Eq. (11). Indeed, if we replace all \( \mu \) therein by \(-i\beta\), the equation reduces into the backward master equation. To some extent, the optimal operator \( \overline{\mathcal{K}}(s'; \mu) \) plays a role analogous to that of \( \overline{\rho}(s) \) in Eq. (18).

In addition to the calculation of the inclusive quantum work, Eq. (32) is also useful in discussing the symmetry of the pdfs of \( H \). On the basis of the quantum jump theory, Horowitz has argued that the Crooks equality \[3, 4\] was held in a specific type of master equations \[22\]. The equality is about the pdfs of the work of the forward and backward QMMEs. To the end, we first denote the CF of the work for the backward Eq. (32) to be \( \tilde{\Phi}(\mu) \). We will show that, if the Hamiltonian is time-reversible at arbitrary time, i.e., \( \Theta H(t) \Theta^\dagger = H(t) \), these two CFs have an important symmetry:

\[
Z(0)\Phi(u) = Z(t_f)\tilde{\Phi}(\nu)
\] (33)

with the parameter \( \nu = i\beta - u \). If one transforms it back into their pdfs, the Crooks equality is recovered \[19\]. We notice that Eq. (33) is exactly the same with that in isolated quantum Hamiltonian systems \[19\]. Because of the duality of the forward and backward equations, for \( \tilde{\Phi}(\mu) \) we may follow the previous argument to introduce an operator \( \overline{\mathcal{K}}(t'; \mu) \) and require

\[
\tilde{\Phi}(\mu) = \frac{1}{Z(t_f)} \text{Tr}[\mathcal{K}(t_f; -\mu)e^{i(\mu + \beta) \tilde{H}(0)}].
\] (34)

Obviously, the operator \( \mathcal{K}(t'; \mu) \) satisfies an evolution equation analogous to Eq. (30) except that all tildes therein are erased and \( s' \) is replaced by \( t' \). The symmetry (33) is essentially attributed to the relation

\[
\tilde{G}(s, 0; \mu)(O) = \Theta \tilde{G}^\ast(t, t_f; -\nu)(\Theta^\dagger O \Theta) \Theta^\dagger,
\] (35)

where \( \tilde{G} \) on the left-hand side is the propagator of Eq. (30), and \( \tilde{G}^\ast \) on another side is the adjoint propagator of the evolution equation of \( \mathcal{K}(t'; \mu) \). Further details about Eq (35) see Appendix II. With these notations, the proof of Eq. (33) is straightforward:

\[
\Phi(\mu)Z(0) = \text{Tr} \left[ \Theta^\dagger \tilde{G}(t_f, 0; \mu)(\tilde{G}(0; \mu) \Theta) e^{iuH(0)} \right] \\
= \text{Tr} \left[ \tilde{G}^\ast(0, t_f; -\nu)(\Theta^\dagger \tilde{K}(0; \mu) \Theta) e^{iuH(0)} \right] \\
= \text{Tr} \left[ \tilde{G}(t_f, 0; -\nu)(e^{iuH(0)}) e^{i\mu H(t_f)} \right] \\
= \tilde{\Phi}(\nu)Z(t_f).
\] (36)

Note that the last equation has used the time-reversible property of the Hamiltonian.

Before closing the theoretical part of this paper, we want to make two comments. The first is about the effect of the initial density matrix. So far, we assumed the initial condition is the thermal state \( \rho_0(0) \). However, the inclusive work \[12\] and the characteristic function \[26\] are always well-defined provided that the initial density matrix is diagonal in the energy representation, namely, \( [\rho(0), H(0)] = 0 \). Under this circumstance, the calculation of the CF based on the evolution Eqs. (28) or (30) is still available. One may see this point more clearly in the proof of Eqs. (24) and (27). The second is about the relation of the current results and those in the isolated quantum Hamiltonian systems. It is apparent that the former reduces into the latter \[14\] if we impose the interaction Hamiltonian \( H_I \) vanishing. Then, all the dissipation terms such as those in Eqs. (11), (9), and (31) will be absent, while the action of the propagator \( G(t_2, t_1)O \) is simplified into \( U(t_2)U^\dagger(t_1)OU(t_1)U^\dagger(t_2) \), where \( U(t) \) is now the unitary time evolution operator of the Hamiltonian \( H(t) \). Moreover, it is well worth emphasizing that for the isolated case, one can safely remove the restriction of the adiabatic evolution of Hamiltonian that is essential for the physical validity of Eq. (11). We do not show this demonstration here \[21, 51\].
VI. EXAMPLE

In this section, we will verify the correctness of the CF method by calculating the pdfs of the inclusive quantum work for a concrete TLS model. Its Hamiltonian is

\[ H(t) = \frac{1}{2} \hbar \omega_0 \sigma_z + g \left( \sigma_+ e^{-i\Omega t} + \sigma_- e^{i\Omega t} \right), \]

and the operator \( A \) is \( \sigma_x \). The time-dependent term may be from the rotating wave approximation of the interaction of the TLS with a driving harmonic field. We simply call \( g \) the field strength. We also emphasize again that the TLS here is not a physical spin. As a result \( \sigma_x \) is time-reversible. In the rest of the paper we choose \( \hbar = 1, k_B = 1, \) and \( \omega_0 = 1 \). The adiabatic eigenvectors and eigenvalues of the Hamiltonian are

\[ | + t \rangle = \cos \frac{\theta}{2} e^{-i\Omega t/2} | + \rangle + \sin \frac{\theta}{2} e^{i\Omega t/2} | - \rangle, \]
\[ | - t \rangle = - \sin \frac{\theta}{2} e^{-i\Omega t/2} | + \rangle + \cos \frac{\theta}{2} e^{i\Omega t/2} | - \rangle, \]

and \( \varepsilon_\pm = \omega / 2 \) with a time-independent \( \omega = \sqrt{1 + 4g^2} \), respectively. Here \( | \pm \rangle \) are the two bases of \( \sigma_z \) and \( \cos \theta = 1 / \omega \).

The Lindblad operators are

\[ A_+(t) = \left( \cos^2 \frac{\theta}{2} e^{i\Omega t} - \sin^2 \frac{\theta}{2} e^{-i\Omega t} \right) | + \rangle \langle -t | + t \langle - | + t \rangle \langle - | - t \rangle \langle - | - t \rangle, \]
\[ A_0(t) = \sin \theta \cos \Omega t (| + t \rangle \langle + | - t \rangle \langle - | - t \rangle). \]

The adiabatic condition here is very simple: \( g \Omega \ll 1 + 4g^2 \). Fig. (2) shows the pdfs of the work at different inverse temperature \( \beta \), the coupling strength \( \kappa \), and the field strength \( g \), where we choose \( \Omega = 0.99 \) and \( t_f = 20\pi / \Omega \). These data are obtained by simulating the quantum jumps and numerically solving the CF with the help of the evolution equation (39), respectively. We see that their agreements are indeed excellent.

These pdfs in Fig. (2) can be qualitatively understood from the point of view of the quantum jump. For the TLS the possible values of the change of the system’s energy are \( \pm \omega \) and 0. If the system is completely isolated, the unique value of the work with nonzero probability is at zero due to the adiabatic condition. Let us see the cases in the right column of the figure. Because of the lower temperature (larger \( \beta \)), we may simply think of that the wave function \( \psi \) of Eq. (1) always starts with the eigenvector \( | -0 \rangle \) [Eq. (39) at time 0]. If the system interacts with the heat bath very weakly, e.g., \( \kappa = 0.03 \), we expect that the probability of zero work still dominates but there are jumps happening in few quantum trajectories. If in a trajectory a rare jump indeed occurs at some time, it is very possible a \( A_- \)-jump and one energy \( \omega \) is released into the heat bath. The reason is that the rate \( \gamma_- \) is far larger than the opposite rate \( \gamma_+ \) at the lower temperature. The work of these trajectories is \( +\omega \). Fig. (2)b shows this scenario. On the other hand, if we keep the same temperature but increase \( \kappa \), the absolute values of these rates increase though their ratio is unchanged. In this situation, not only does the population of trajectories with jumps become larger, but the frequency of the jumps in a same trajectory increases. Accordingly, the probability of zero work shall considerably decrease while the probabilities of the work with larger positive values present. This is what we see in Fig. (2)d. The above arguments also imply that, if we increase the time \( t_f \), we shall see the movements of these pdfs toward the right-hand side. We indeed observe this trend in calculations (data not shown here). Finally, in Fig. (2)f we see that the probabilities of the negative work almost vanish. This is due to the fact that the larger field strength \( g \) leads into the negligible \( \gamma_+ \). Hence, the \( A_+ \)-jumps that are responsible for the negative work are heavily inhibited. For the cases in the left column of the figure, analogous analysis can be carried out. Due to the higher temperature (smaller \( \beta \)), however, two additional factors must be taken into account. One is that the contribution of the initial state at the eigenvector \( | +0 \rangle \) becomes significant now. Another is that the two rates \( \gamma_+ \) and \( \gamma_- \) are comparable, which results in the increasing contributions of the \( A_+ \)-jumps. This is true even at larger \( g \).

VII. CONCLUSION.

In this work, we have developed the CF method to calculate the pdfs of the inclusive quantum work for the adiabatic QMMEs. We showed that this method is also useful in discussing the symmetric properties of the pdfs. Hence, the CF method provides us with an alternative way of studying the quantum work besides the simulation of quantum jumps. The quantum master equations and the quantum-jump theory were known to be complementary either in the physical interpretations or in the practical calculations. Our efforts here and before [26] may be regarded as a concrete realization of the spirit in the specific theme. Although the adiabatic quantum master equation and
FIG. 2. The pdfs of the inclusive work for the TLS. The bars are calculated by simulating the quantum trajectories, while the solid bold lines are obtained by the CF method. The unit of the work $W$ is $\omega$. In these panels the thin dash lines at zero positions guide for eyes.

the equations that are about the systems driven by weak fields are two often used time-dependent QMMEs, e.g., in the intriguing quantum heat engines, they do not definitely cover all situations. For instance, other interesting master equations have been proposed for the dissipative systems under a intensive and fast varying field. It shall be interesting to investigate in future whether the quantum works can be physically defined and what methods can effectively calculate them if they exist.

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For the first equation we write down the explicit expression of its left-hand side,

\[ E[W] = E[\varepsilon(t_f)] - E[\varepsilon(0)] - \int_{t_0}^{t_f} \hbar \omega_t E[dN_+(t_1)] + \int_{t_0}^{t_f} \hbar \omega_t E[dN_-(t_1)]. \]  

(42)

On the basis of the following relations [31],

\[ E[\varepsilon(t)] = \text{Tr}[H(t)\rho(t)], \]

(43)

\[ E[dN_{\pm}(t)] = \gamma_{\pm}(\omega_t)\text{Tr}[A_{\pm}(t)A_{\pm}(t)\rho(t)]dt, \]  

(44)

Eq. (42) can be rewritten as

\[ E[W] = \text{Tr}[H(t_f)\rho(t_f)] - \text{Tr}[H(0)\rho(0)] + \int_{t_0}^{t_f} d\tau \hbar \omega_t \text{Tr}[(\gamma_{-}(\omega_t)A_{+}(t_1)A_{-}(t_1) - \gamma_{+}(\omega_t)A_{-}(t_1)A_{+}(t_1))\rho(t_1)] \]

\[ = \int_{t_0}^{t_f} dt_1 \frac{d}{dt_1} \text{Tr}[H(t_1)\rho(t_1)] - \int_{t_0}^{t_f} dt_1 \text{Tr}[D_t^* [H(t_1)]\rho(t_1)] \]

\[ = \int_{t_0}^{t_f} dt_1 \text{Tr}[\partial_t H(t_1)\rho(t_1)], \]  

(45)

where \( D_t^* \) is the adjoint superoperator of \( D_t \) in Eq. (42). We see that the last two equations are just the first law of thermodynamics for the adiabatic QMME (11) [39]. The derivation of Eq. (25) is more complicated. We first write the explicit form of the left-right hand of the equation:

\[ E[W^2] = E\left[(\varepsilon(t_f) - \varepsilon(0))^2\right] + E\left[\left(\int_{t_0}^{t_f} dt_1 \hbar \omega_t dN_-(t_1) - \int_{t_0}^{t_f} dt_2 \hbar \omega_t dN_+(t_2)\right)^2\right] \]

\[ + 2E\left[(\varepsilon(t_f) - \varepsilon(0))\left(\int_{t_0}^{t_f} dt_1 \hbar \omega_t dN_-(t_1) - \int_{t_0}^{t_f} dt_2 \hbar \omega_t dN_+(t_2)\right)\right]. \]  

(46)

In order to express these terms into the multiple time correlation functions of operators, which is two time points here, we need apply the following relations:

\[ E[\varepsilon^2(t)] = \text{Tr}[H^2(t)\rho(t)], \]

(47)

\[ E[\varepsilon(t)\varepsilon(0)] = \text{Tr}[H(t)G(t,0)H(0)\rho(0)], \]

(48)

\[ E[\varepsilon(t)\varepsilon(t) dN_{\pm}(t)] = \gamma_{\pm}(\omega_t)\text{Tr}[H(t)G(t,0)A_{\pm}(t)\rho(t)A_{\mp}(t)dt], \]

(49)

\[ E[\varepsilon(0)dN_{\pm}(t)] = \gamma_{\pm}(\omega_t)\text{Tr}[A_{\mp}(t)A_{\pm}(t)G(t,0)H(0)\rho(0)]dt, \]

(50)

and the other three correlation functions about \( E[dN_{\pm}(t_1)dN_{\pm}(t_2)] \) that have been given in our previous study [26]. Substituting them in Eq. (45) and doing a careful algebra, we may arrive at the right-hand side of Eq. (25). Some details are almost parallel with what we did in the case of quantum BKE [26].

**APPENDIX II: PROOF OF EQ. (35)**

This relationship of the propagator \( \tilde{G}(s,0;\mu) \) and the adjoint propagator \( \tilde{G}^*(t,t_f;-\nu) \) is the consequence of the characteristic of their generators,

\[ \tilde{L}_s(\mu)(O) = \Theta \tilde{L}^*_t(-\nu)[\Theta^\dagger O \Theta]\Theta^\dagger. \]  

(51)

\( \tilde{L}_s(\mu) \) has been given in Eq. (51). We need to explicitly write out another only:

\[ \tilde{L}^*_t(\mu)O = \frac{i}{\hbar}[H(t),O] + \sum_{\alpha=\pm} \gamma_{\alpha}(\omega_t)[e^{\alpha i\hbar \omega_t}A_{\alpha}(t)O A_{\alpha}^\dagger(t) - \frac{1}{2}\{A_{\alpha}^\dagger(t)A_{\alpha}(t),O\}]

\[ + \gamma_0[A_0(t)O A_{\alpha}^\dagger(t) - \frac{1}{2}\{A_{\alpha}^\dagger(t)A_0(t),O\}]. \]  

(52)
Then the verification of Eq. (51) is straightforward. Note that $\tilde{L}_t^\dagger(\mu)$ recovers the adjoint superoperator $L_t^\dagger$ in Eq. (21) if $\mu$ here is replaced by $-i\beta$. 

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