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

Fei Liu[*]

School of Physics and Nuclear Energy Engineering, Beihang University, Beijing 100191, China
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We present a characteristic function method to calculate the probability density functions of the inclusive work in adiabatic two-level quantum Markovian master equations. These systems are steered by some slowly varying parameters and the dissipations may depend on time. Our theory is based on the interpretation of the quantum jump for the master equations. In addition to the calculation, we also find that the fluctuation properties of the work can be described by the symmetry of the characteristic functions, which is exactly the same as in the case of isolated systems. A periodically driven two-level model is used to demonstrate the method.

I. INTRODUCTION

In the past decade, extending classical work equalities [1–4] into the nonequilibrium quantum regime has attracted intensive interest [1,5–30]. With the growing consensus about the definitions of work and their equality in isolated quantum systems [14], recently some attention has been devoted to quantum Markovian master equations (QMMEs) [20–30]. Among this, the notion of the quantum jump [31–34] used in the quantum optics literature was introduced. As one of the statistical interpretations of the master equations having the Lindblad form [35–37], the quantum jump not only provides physically reasonable definitions of work for these quantum systems, but also makes quantum extensions of the work equality straightforward. For instance, combining this notion with the scheme of two energy measurements [5,15], Horowitz [25] proved a quantum Jarzynski equality (QJE) for a specific type of master equation. These equations were assumed to have instantaneous thermal equilibrium solutions. With a similar idea Hekking and Pekola [27] and we [30] presented a quantum Bochkov-Kuzovlev equality (BKE) [1] for another type of master equation. Unlike those in Ref. [25], the systems of the latter are driven by weak external fields and their dissipations are time independent.

Although these achievements are significant, we note that most of them focused on the formal derivations of the work equalities in the various QMMEs; few [27,30] investigated the calculations of the probability density functions (PDFs) of the work. In our opinion, this kind of effort is essential since the PDF of work is a fundamental quantity in the thermodynamics of finite quantum systems [9]. The work equality is only one of the characteristics of work under specific conditions [14,38]. A direct method of calculating work is by simulation [27]. By repeatedly generating quantum jumps [32–34], one may readily construct statistical histograms of work. However, it is inconvenient for theoretical investigations. For instance, a simulation does not provide us with a relation between the moment of the work and the master equation. Additionally, it also bears the errors of statistical sampling. Very recently, in a specific type of master equation an alternative method was developed by us [30]. It

is based on solving the characteristic function (CF) of the exclusive work [39]. This method not only presents closed expressions for the moments of the work, but also is simple in numerical realization. Due to these attractive features, in this paper we try to extend the previous CF method to the case of inclusive work [39] in quantum adiabatic master equations [40–44]. These equations describe the dynamics of dissipated systems that are adiabatically steered by some external parameters. They have often been utilized to model the decoherence effects of thermal environments in quantum adiabatic computations [45–49].

The paper is organized as follows. In Sec. II we briefly review a generic two-level adiabatic QMME and its quantum jump interpretation. The essential notations are set up. In Sec. III we define the backward master equation of the forward equation. In Sec. IV we prove that the QJE in the same forward master equation possesses two different expressions. On the basis of this observation, in Sec. V we present the CF method to calculate the PDFs of the inclusive work. In Sec. VI a simple two-level model is used to illustrate our method. Section VII concludes this paper. Some key points in the formal derivations are shown in Appendices A and B.

II. TWO-LEVEL ADIABATIC QMME AND QUANTUM JUMP INTERPRETATION

For simplicity in notation, throughout this paper we employ a generic two-level adiabatic master equation to develop our theory. The most general form of the equation can be found in Ref. [42]. Although we will use the Pauli matrices, we do not consider physical spins. In the time interval $(0,t_f)$, the two-level system (TLS) evolves under an adiabatically varying Hamiltonian $H(t)$. Meanwhile, it exchanges energy with a heat bath at the inverse temperature β. The time dependence is usually implemented via some external parameters. Here we did not explicitly write them out. We assume the interaction term between the system and the heat bath to be $H_I = A \otimes B$. Under the adiabatic condition, the weak-coupling Markovian approximation, and the secular approximation, the equation of motion of the reduced density matrix $\rho(t)$ for the system is [40–44]

$$\partial_t \rho(t) = \mathcal{L}_t \rho(t) = -\frac{i}{\hbar}[H(t),\rho(t)] + D_t[\rho(t)]. \quad (1)$$

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[*]feiliu@buaa.edu.cn

The time-dependent dissipation term is

$$D_t[\rho] = \sum_{\alpha=\pm} \gamma_\alpha(\omega_t) \left[A_\alpha(t)\rho A_\alpha^\dagger(t) - \frac{1}{2}\{A_\alpha^\dagger(t)A_\alpha(t),\rho\} \right]$$
$$+ \gamma_0 \left[A_0(t)\rho A_0^\dagger(t) - \frac{1}{2}\{A_0^\dagger(t)A_0(t),\rho\} \right]. \quad (2)$$

The rates $\gamma_\pm(\omega)$ and γ_0 equal $\Gamma(\mp\omega)$ and $\Gamma(0)$, respectively, where $\Gamma(\omega)=\int_{-\infty}^{+\infty} d\tau e^{i\omega\tau}\langle B(\tau)B(0)\rangle_{eq}$ and the average is associated with the equilibrium heat bath. The Lindblad operators $A_\pm(t)$ and $A_0(t)$ are

$$|\varepsilon_\pm(t)\rangle\langle\varepsilon_\pm(t)|A|\varepsilon_\mp(t)\rangle\langle\varepsilon_\mp(t)| \quad (3)$$

and

$$\sum_{\alpha=\pm} |\varepsilon_\alpha(t)\rangle\langle\varepsilon_\alpha(t)|A|\varepsilon_\alpha(t)\rangle\langle\varepsilon_\alpha(t)|, \quad (4)$$

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

$$[H(t),A_\pm(t)] = \pm\hbar\omega_t A_\pm(t), \quad (5)$$

and $[H(t),A_0(t)] = 0$, where $\hbar\omega_t = \varepsilon_+(t)-\varepsilon_-(t)$. The crucial assumption on which this paper depends is the instantaneous detailed balance condition $\gamma_+(\omega_t) = \gamma_-(\omega_t)e^{-\beta\hbar\omega_t}$. In addition, we also specify the correlation function of the heat bath to be an Ohmic spectral density [50], i.e., $\gamma_0 = \kappa/\hbar\beta$ and $\gamma_-(\omega) = \kappa\omega/(1 - e^{-\beta\hbar\omega})$, where κ is the coupling strength. The structure of Eq. (1) and the instantaneous detailed balance condition ensure that the TLS always has an instantaneous thermal state

$$\rho_{eq}(t) = \sum_{\alpha=\pm} \frac{e^{-\beta\varepsilon_\alpha(t)}}{Z(t)}|\varepsilon_\alpha(t)\rangle\langle\varepsilon_\alpha(t)|$$
$$= \sum_{\alpha=\pm} p_\alpha^{eq}(t)|\varepsilon_\alpha(t)\rangle\langle\varepsilon_\alpha(t)|, \quad (6)$$

where $Z(t) = \text{Tr}[e^{-\beta H(t)}]$ is the instantaneous partition function at time t. Finally, we specify the initial density matrix to be $\rho_{eq}(0)$ unless otherwise stated. The conditions for the physical validity of Eq. (1) have been rigorously analyzed [42,51].

According to the quantum jump theory [32–34], the density matrix $\rho(t)$ can be interpreted as a statistical average of the wave function $\psi(t)$. This wave function varies in the Hilbert space of the TLS with alternatively deterministic continuous evolution and stochastic jumps. Its deterministic equation of motion is

$$\partial_t\psi(t) = -\frac{i}{\hbar}\hat{H}(t)\psi(t)$$
$$= -\frac{i}{\hbar}H(t)\psi(t)$$
$$- \frac{1}{2}\left(\sum_{\alpha=\pm}\gamma_\alpha(\omega_t)A_\alpha^\dagger(t)A_\alpha(t) + \gamma_0 A_0^\dagger(t)A_0(t)\right)\psi(t). \quad (7)$$

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 call them $A_\pm$ and A_0 jumps,

respectively. The probabilities of these jumps are proportional to $\gamma_\pm(\omega_t)\|A_\pm(t)\psi(t)\|^2$ and $\gamma_0\|A_0(t)\psi(t)\|^2$, respectively. Since the wave function $\psi(t)$ can always be written as $\sum_{\alpha=\pm} c_\alpha(t)|\varepsilon_\alpha(t)\rangle$, after the jump the former two states are indeed $|\varepsilon_\pm(t)\rangle$ and their jumping probabilities are proportional to $\gamma_\pm(\omega_t)|c_\mp(t)|^2$. From the energetic point of view, $A_\pm$ jumps accompany an absorption and a release of energy $\hbar\omega_t$ by the system from and to the heat bath, respectively. In contrast, the A_0 jump induces only changes of the local phases of the wave function. Given the above explanations, the probability of observing a trajectory in the time interval $(0,t)$ whose initial state is $|\psi_0\rangle$ undergoes N jumps at increasing times t_i $(i = 1,\ldots,N)$ with the order of jumps $(A_{\alpha_1},\ldots,A_{\alpha_N})$ is

$$\prod_{i=N}^{1} dt_i \prod_{i=N}^{1} \gamma_{\alpha_i}\|\mathcal{L}_N(t,0)|\psi_0\rangle\|^2$$
$$= \prod_{i=N}^{1} dt_i \prod_{i=N}^{1} \gamma_{\alpha_i}\|U(t,t_N)A_{\alpha_N}(t_N)\cdots U(t_2,t_1)$$
$$\times A_{\alpha_1}(t_1)U(t_1,0)|\psi_0\rangle\|^2. \quad (8)$$

Here α_i equals $\pm$ or 0. We did not explicitly write out ω_{t_i} in the rates $\gamma_\pm$. Additionally, the notation U is the *nonunitary* time evolution operator of Eq. (7) in a certain time interval, e.g., $U(t_2,t_1) = \mathcal{T}_-\exp[-\frac{i}{\hbar}\int_{t_1}^{t_2} d\tau \hat{H}(\tau)]$, where $\mathcal{T}_-$ denotes the chronological time-ordering operator. With the probability density of the quantum trajectory and doing a summation over all trajectories, one may calculate the density matrix from the wave function as $\rho(t) = E\left[|\psi(t)\rangle\langle\psi(t)|\right]$ [32–34].

III. BACKWARD ADIABATIC QMMES

The work equalities are intimately related to the symmetry of the system and its time reversal [3,4,14,38]. As a preliminary to the following discussion, we introduce the time reversal of the forward Eq. (1), or the backward adiabatic QMME. First we define $\widetilde{H}(s) = \Theta H(t)\Theta^\dagger$ as the time-reversed Hamiltonian, where another time parameter $s = t_f - t$, and Θ is the time-reversal operator. Throughout this paper, we use the notations with a tilde to denote the meanings of the quantities under time reversal. Obviously, the eigenvectors $|\widetilde{\varepsilon}_\alpha(s)\rangle$ and eigenvalues $\widetilde{\varepsilon}_\alpha(s)$ of $\widetilde{H}(s)$ equal $\Theta|\varepsilon_\alpha(t)\rangle$ and $\varepsilon_\alpha(t)$, respectively. Given that the interaction Hamiltonian H_I is time reversible, which we always assume here, we introduce the backward master equation

$$\partial_s\widetilde{\rho}(s) = \widetilde{\mathcal{L}}_s\widetilde{\rho}(s) = -\frac{i}{\hbar}[\widetilde{H}(s),\widetilde{\rho}(s)] + \widetilde{D}_s[\widetilde{\rho}(s)]. \quad (9)$$

The dissipation term is

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

The time-reversed rates and Lindblad operators have simple connections with the original ones: $\widetilde{\gamma}_\alpha(\widetilde{\omega}_s) = \gamma_\alpha(\omega_t)$, $\widetilde{\gamma}_0 = \gamma_0$, $\widetilde{A}_\pm(s) = \Theta A_\pm(t)\Theta^\dagger$, and $\widetilde{A}_0(s) = \Theta A_0(t)\Theta^\dagger$. Comparing Eq. (9) with (1), we see that the former may be 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 a quantum jump as well. For instance, the deterministic evolution equation for Eq. (9) is

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

where $\hat{\widetilde{H}}$ is analogous to $\hat{H}(t)$ in Eq. (7) except that the operators and rates therein are replaced by their time-reversed quantities.

IV. TWO EXPRESSIONS FOR THE QJE

In order to construct the CF method for the inclusive work, we first prove the equivalence of two QJEs in the same master equation (1). They were proposed by Horowitz [25] and Chetrite and Mallick [26], respectively. The latter equality is an abstract "book-keeping" of a sum of multiple time correlation functions of the operators. Interestingly, the notions of the quantum jump and energy measurements were not involved. Following our previous convention [30], we call them the *c*- and *q-number* QJEs, respectively. So far, their relation has not been clarified. The reader will see that the equivalent demonstration indeed provides us with a shortcut toward an important evolution equation that can assist the calculation of the CFs.

A. *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 $|\varepsilon_\alpha(t')\rangle$. We begin with a quantum trajectory of Eq. (1) starting with this state. If we record the order of jumps $(A_{\alpha_1}, \ldots, A_{\alpha_N})$ at later times $(t_1, \ldots, t_N)$, 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 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 time τ. Note that N_0, the number of A_0 jumps, is not involved since they do not contribute any energy changes. Now we are concerned with the following equation:

$$e^{-\beta W(t')} \left[\prod_{i=N}^{1} dt_i \prod_{i=N}^{1} \gamma_{\alpha_i} \| \langle \varepsilon_\delta(t_f) | \mathcal{L}_N(t_f, t') | \varepsilon_\alpha(t') \rangle \|^2 \right] p_\alpha^{eq}(t'). \tag{13}$$

According to Eq. (8), the whole term in the above 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 [24,25]. We first notice that the terms in the exponential function of the work can be combined into rates using the instantaneous detailed balance condition. Then we

rewrite the equation as

$$\frac{Z(t_f)}{Z(t')} \left[\prod_{i=1}^{N} dt_i \prod_{i=1}^{N} \gamma_{\widetilde{\alpha}_i} \| \langle \varepsilon_\alpha(t') | \Theta^\dagger \widetilde{\mathcal{L}}_N(s', 0) \Theta | \varepsilon_\delta(t_f) \rangle \|^2 \right]$$
$$\times p_\delta^{eq}(t_f), \tag{14}$$

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

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

We immediately see that the term in the second set of square brackets is just $\widetilde{A}_{\widetilde{\alpha}_1}(s_N)$ of the backward Eq. (9). Here we define $s_j + t_i = t_f$ and $i + j = N + 1$. Note that the $\widetilde{A}_{\widetilde{\alpha}_1}$ and A_{α_1} jumps are opposite unless $\alpha_1 = 0$. Moreover, we may check that the term in the first set of square brackets is the nonunitary time evolution operator $\widetilde{U}(s', s_N)$ of Eq. (11) in the time interval (s_N, s'). For the remaining terms in Eq. (15) these two observations are true as well. Noting that $\widetilde{\gamma}_{\widetilde{\alpha}_i}(\widetilde{\omega}_{s_i}) = \gamma_{\widetilde{\alpha}_i}(\omega_{t_j})$, we finally find that the whole term in the square brackets of Eq. (14) is nothing but the conditional probability of a quantum trajectory for the backward master equation (9): its state at time 0 is $\Theta | \varepsilon_\delta(t_f) \rangle$, the order of jumps is $(\widetilde{A}_{\widetilde{\alpha}_N}, \ldots, \widetilde{A}_{\widetilde{\alpha}_1})$ at times $(s_1, \ldots, s_N)$, and the energy eigenvector measured at the final time s' is $\Theta | \varepsilon_\alpha(t') \rangle$. Figure 1 is a schematic diagram of two time-reversed quantum trajectories.

Now we perform 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. (14), we establish an important equation,

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

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

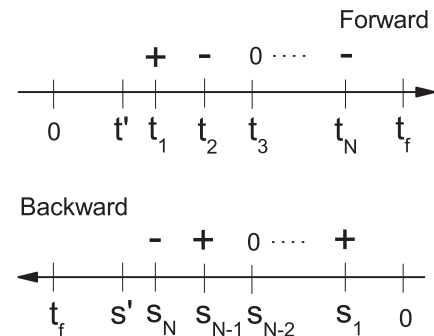$$E[e^{-\beta W(0)}] = e^{-\beta \Delta G}, \tag{17}$$

FIG. 1. A quantum jump trajectory of the forward adiabatic QMME and its time reversal. The arrows indicate the directions of time. The symbols $\pm$ and 0 represent the $A_\pm$ and A_0 jumps, respectively.

where $\beta\Delta G = \ln Z(t_f) - \ln Z(0)$. The reader is reminded that the initial condition of the forward Eq. (1) must be the thermal state, which explains 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:

$$R(t',t_f)\rho_{eq}(t') = \Theta^{\dagger}\widetilde{\rho}(s')\Theta. \tag{18}$$

Note that its validity has nothing to do with the quantum jump provided $\widetilde{\rho}(s')$ and $\rho_{eq}(t')$ are well defined. Writing Eq. (18) in the energy representation and comparing it with Eq. (16), we have

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

Obviously, the operator $R(t',t_f)$ possesses all characteristics that the E_{α} term has. In the following we pay attention to the general properties of $R(t',t_f)$ and temporarily set aside the quantum jump. Substituting Eq. (18) into Eq. (9), we are able to obtain an evolution equation about $R(t',t_f)$ with respect to t':

$$\partial_{t'}R(t',t_f) = -\mathcal{L}_{t'}^{\star}R(t',t_f) - R(t',t_f)\partial_{t'}\rho_{eq}(t')\rho_{eq}^{-1}(t'), \tag{20}$$

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

$$\mathcal{L}_{t'}^{\star}O = \frac{i}{\hbar}[H(t'),O]$$
$$+ \sum_{\alpha=\pm}\gamma_{\alpha}(\omega_{t'})\left[A_{\alpha}^{\dagger}(t')OA_{\alpha}(t') - \frac{1}{2}\{A_{\alpha}^{\dagger}(t')A_{\alpha}(t'),O\}\right]$$
$$+ \gamma_0\left[A_0^{\dagger}(t')OA_0(t') - \frac{1}{2}\{A_0^{\dagger}(t')A_0(t'),O\}\right]. \tag{21}$$

To arrive at Eq. (20), we applied the instantaneous detailed balance condition again. Here we must emphasize that this result is not affected by the initial conditions of the forward and backward master equations. In addition, Eq. (20) is a terminal value problem, i.e., $R(t_f,t_f) = I$, the identity operator. Introducing the adjoint propagator $G^{\star}(t_1,t_2) = \mathcal{T}_+\exp[\int_{t_1}^{t_2}d\tau\mathcal{L}_{\tau}^{\star}]$ [33] ($t_1 < t_2$), where $\mathcal{T}_+$ denotes the antichronological time-ordering operator, we may have a formal solution of Eq. (20) written as the celebrated Dyson series [26,30,52]. Choosing $t' = 0$ and taking traces on the two sides of Eq. (18), we obtain the *q-number* QJE [26,52] for the same master equation (1),

$$\left\langle\mathcal{T}_+\exp\left[\int_0^{t_f}d\tau\mathcal{W}(\tau)\right]\right\rangle = e^{-\beta\Delta G}. \tag{22}$$

Here we defined an operator $\mathcal{W}(\tau) = \partial_{\tau}e^{-\beta H(\tau)}e^{\beta H(\tau)}$. It is worth pointing out that the "average" $\langle\ \rangle$ above is only a shorthand notation [26]. Indeed, its explicit expression is a sum of infinite terms of multiple time correlation functions of

the operators [33]:

$$1 + \left\langle\int_0^{t_f}dt_1\mathcal{W}(t_1)\right\rangle + \left\langle\int_0^{t_f}dt_1\int_{t_1}^{t_f}dt_2\mathcal{W}(t_2)\mathcal{W}(t_1)\right\rangle + \cdots$$
$$= 1 + \int_0^{t_f}dt_1\mathrm{Tr}[\mathcal{W}(t_1)G(t_1,0)\rho_{eq}(0)] + \int_0^{t_f}dt_1\int_{t_1}^{t_f}dt_2\mathrm{Tr}$$
$$\times[\mathcal{W}(t_2)G(t_2,t_1)\mathcal{W}(t_1)G(t_1,0)\rho_{eq}(0)] + \cdots, \tag{23}$$

where $G(t_2,t_1) = \mathcal{T}_-\exp[\int_{t_1}^{t_2}d\tau\mathcal{L}_{\tau}]$ is the propagator of Eq. (1). 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 QJEs. An alternative proof is to expand the exponential functions in Eqs. (17) and (22) as a series in the inverse temperature β and to check whether their coefficients are equal. To implement this scheme, one has to first know the correlation functions of the quantum jumps among different times. Fortunately, they have been given previously [34]. Here we list the final results for the first two coefficients which are indeed the first two moments of the inclusive work:

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

$$E[W^2] = 2\int_0^{t_f}dt_1\int_{t_1}^{t_f}dt_2\langle\partial_{t_2}H(t_2)\partial_{t_1}H(t_1)\rangle$$
$$+ \int_0^{t_f}dt_1\langle[H(t_1),\partial_{t_1}H(t_1)]\rangle. \tag{25}$$

Note that the second term in the second equation is a pure quantum effect. We leave their derivations to Appendix A.

V. CHARACTERISTIC FUNCTION OF INCLUSIVE WORK

In the preceding discussion, we clearly see that the PDF of the inclusive work (12) can be constructed using quantum jump simulation [33,34]. On the contrary, we do not gain such an impression in the case of the q-number equality. For the latter, a possible way is to calculate all the moments of the work using equations like Eqs. (24) and (25) and then to convert them to the PDFs. However, for the higher moments, as well as higher-dimensional integrations being involved, their connections with the multiple time correlation function will become extremely complicated. Hence, this method 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 μ is a real number. After solving the CF, the PDF is obtained by performing an inverse Fourier transform of $\Phi(\mu)$. At first glance, Eq. (26) does not show apparent advantages. However, the CF may be regarded as the left-hand side of the QJE (17) except that β therein is replaced by an *imaginary* inverse temperature $-i\mu$. 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 as

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

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

$$\partial_{t'} K(t',t_f;\mu) = -\mathcal{L}_{t'}^\star K(t',t_f;\mu) - K(t',t_f;\mu)\partial_{t'} e^{i\mu H(t')}$$
$$\times\, e^{-i\mu H(t')}, \tag{28}$$

and the terminal condition is $K(t_f,t_f;\mu) = I$. This is the central result of this paper.

At this stage we have achieved the goal of calculating the PDF of the work by solving Eq. (28) rather than simulating the quantum trajectories. In practice, however, it is inconvenient to compute the exponential functions of the Hamiltonian operator; see the last term in the above equation. In addition, this is a terminal value problem rather than the conventional initial value problem. These two undesirable features may be remedied by introducing another "better" operator,

$$\widetilde{\mathcal{K}}(s';\mu) = \Theta K(t',t_f;\mu) e^{i\mu H(t')}\Theta^\dagger. \tag{29}$$

After simple algebra we have

$$\partial_{s'}\widetilde{\mathcal{K}}(s';\mu) = \widetilde{\mathcal{L}}_{s'}(\mu)\widetilde{\mathcal{K}}(s';\mu), \tag{30}$$

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

$$\widetilde{\mathcal{L}}_s(\mu)O = -\frac{i}{\hbar}[\widetilde{H}(s),O] + \sum_{\alpha=\pm}\widetilde{\gamma}_\alpha(\widetilde{\omega}_s)$$
$$\times\left[e^{\alpha i\mu\hbar\widetilde{\omega}_s}\widetilde{A}_\alpha^\dagger(s)O\widetilde{A}_\alpha(s) - \frac{1}{2}\{\widetilde{A}_\alpha^\dagger(s)\widetilde{A}_\alpha(s),O\}\right]$$
$$+ \widetilde{\gamma}_0\left[\widetilde{A}_0^\dagger(s)O\widetilde{A}_0(s) - \frac{1}{2}\{\widetilde{A}_0^\dagger(s)\widetilde{A}_0(s),O\}\right]. \tag{31}$$

Accordingly, Eq. (27) is slightly modified to

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

The second equation is because $\mathrm{Tr}[\Theta^\dagger O\Theta] = \mathrm{Tr}[O^\dagger]$. We see that Eq. (31) is very close to Eq. (9). Indeed, if we replace all μ therein by $-i\beta$, the former will be reduced to the latter.

In addition to the calculation, Eq. (32) is also useful in discussing the symmetry of the PDFs of the inclusive work. On the basis of the quantum jump theory, Horowitz has argued that the Crooks equality [3,4] was maintained in a specific type of master equation [25]. The equality concerns the PDFs of the work for the forward and backward QMMEs. To the end, we first denote the CF for Eq. (9) as $\widetilde{\Phi}(\mu)$. We will show that, if the Hamiltonian is time reversible at an arbitrary time, i.e., $\Theta H(t)\Theta^\dagger = H(t)$, these two CFs satisfy an important symmetry,

$$Z(0)\Phi(u) = Z(t_f)\widetilde{\Phi}(v), \tag{33}$$

where $v = i\beta - u$. If one transforms it back into the PDFs, the Crooks equality will be recovered [14]. We notice that Eq. (33) is exactly the same as that in isolated quantum systems [14]. Because of the duality of the forward and backward equations, for $\widetilde{\Phi}(\mu)$ we may follow the previous argument to introduce

an operator $\mathcal{K}(t';\mu)$ and require

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

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

$$\widetilde{G}(s,0;\mu)(O) = \Theta\breve{G}^\star(t,t_f;-v)(\Theta^\dagger O\Theta)\Theta^\dagger, \tag{35}$$

where $\widetilde{G}$ on the left-hand side is the propagator of Eq. (30), and $\breve{G}^\star$ on the other side is the adjoint propagator of the evolution equation of $\mathcal{K}(t';\mu)$. Appendix B presents further details about this relation. With these notations proving Eq. (33) is straightforward:

$$\Phi(\mu)Z(0) = \mathrm{Tr}[\Theta^\dagger\widetilde{G}(t_f,0;\mu)(\breve{\mathcal{K}}(0;\mu))\Theta e^{ivH(0)}]$$
$$= \mathrm{Tr}[\breve{G}^\star(0,t_f;-v)(\Theta^\dagger\breve{\mathcal{K}}(0;\mu)\Theta)e^{ivH(0)}]$$
$$= \mathrm{Tr}[\breve{G}(t_f,0;-v)(e^{ivH(0)})e^{i\mu H(t_f)}]$$
$$= \widetilde{\Phi}(v)Z(t_f). \tag{36}$$

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

Before closing the theoretical part of this paper, we want to make several comments. The first is the effect of the initial density matrix. So far, we have always assumed the initial reduced density matrix $\rho(0)$ to be the thermal state $\rho_{eq}(0)$. 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 using the evolution equation (28) or (30) is still available. One may see this point more clearly in term of the proof of Eqs. (24) and (25). The second is the relation between the current results and those in isolated quantum Hamiltonian systems. Obviously, the former reduces to the latter [14] if we impose vanishing of the interaction Hamiltonian H_I. Then, all the dissipation terms such as those in Eqs. (1), (9), and (31) will be absent. Meanwhile, the action of the propagator $G(t_2,t_1)$ on an operator O is simplified to $U(t_2)U^\dagger(t_1)OU(t_1)U^\dagger(t_2)$, where $U(t)$ is now the *unitary* time evolution operator of $H(t)$. Moreover, it is well worth emphasizing that for the isolated case, one can remove the restriction of the adiabatic evolution of Hamiltonian that is essential for the physical validity of Eq. (1). We do not pursue further details here [16,53]. Finally, Talkner *et al.* [12] have used another characteristic function method to prove the validity of the JE and Crooks' equality for very general open quantum systems. Except for the weak-coupling approximation, the dynamics of the system therein is not required to be Markovian and the external parameters may vary arbitrarily. There are two key ingredients in their method. One is the unitary evolution of the composition of the system and the heat bath. The other is the simultaneous measurement of the energies of the system and the heat bath at the beginning and the end of the process. The theory is fully microscopic while our starting point is the effective dynamics of the reduced system. The advantage of the latter is that it is closer to the real situation in laboratories. Although in

principle the results of Talkner *et al.* [12] cover what we obtained here if the additional requirements are imposed, we do not think that establishing this connection would be simple from the technical perspective; see the analogous efforts in Refs. [13,18].

VI. EXAMPLE

In this section, we will illustrate the CF method by calculating the PDFs of the inclusive work in a simple TLS model. Its Hamiltonian is

$$H(t) = \frac{1}{2}\hbar\omega_0\sigma_z + g(\sigma_+ e^{-i\Omega t} + \sigma_- e^{i\Omega t}), \quad (37)$$

and the operator A is σ_x. The time-dependent term may be from the rotating-wave approximation of the interaction of the TLS with a driving harmonic field [33]. We simply call g the field strength. We emphasize again that the TLS is not a physical spin. As a result σ_x is time reversible. For the sake of simplicity, we let $\hbar = 1$, $k_B = 1$, and $\omega_0 = 1$. The adiabatic eigenvectors and eigenvalues of the Hamiltonian are

$$|+t\rangle = \cos\frac{\theta}{2}e^{-i\Omega t/2}|+\rangle + \sin\frac{\theta}{2}e^{i\Omega t/2}|-\rangle, \quad (38)$$

$$|-t\rangle = -\sin\frac{\theta}{2}e^{-i\Omega t/2}|+\rangle + \cos\frac{\theta}{2}e^{i\Omega t/2}|-\rangle, \quad (39)$$

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

$$A_+(t) = \left(\cos^2\frac{\theta}{2}e^{i\Omega t} - \sin^2\frac{\theta}{2}e^{-i\Omega t}\right)|+t\rangle\langle -t|, \quad (40)$$

$$A_0(t) = \sin\theta\cos\Omega t\,(|+t\rangle\langle +t| - |-t\rangle\langle -t|). \quad (41)$$

The adiabatic condition is very simple: $g\Omega \ll 1 + 4g^2$. Figure 2 shows the PDFs of the inclusive work at different inverse temperatures β, the coupling strength κ, and the field strength g. We chose $\Omega = 0.99$ and $t_f = 20\pi/\Omega$ or 10 cycles. These data are obtained by simulating the quantum jumps and numerically solving the CF with the assistance of the evolution equation (30), respectively. We see that their agreement is 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, under the adiabatic condition the unique value of the work with nonzero probability is zero. Let us inspect the cases in the right column of the figure. Because of the lower temperature (larger β), we consider that the wave function ψ of Eq. (7) 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 possibly an A_- jump and an energy ω is released into the heat bath. The reason is that the rate γ_- is far larger than the opposite rate γ_+ at the lower temperature. The work of these trajectories is $+\omega$. Figure 2(b) shows this scenario. On the other hand, if we increase κ but keep the same temperature, the absolute values
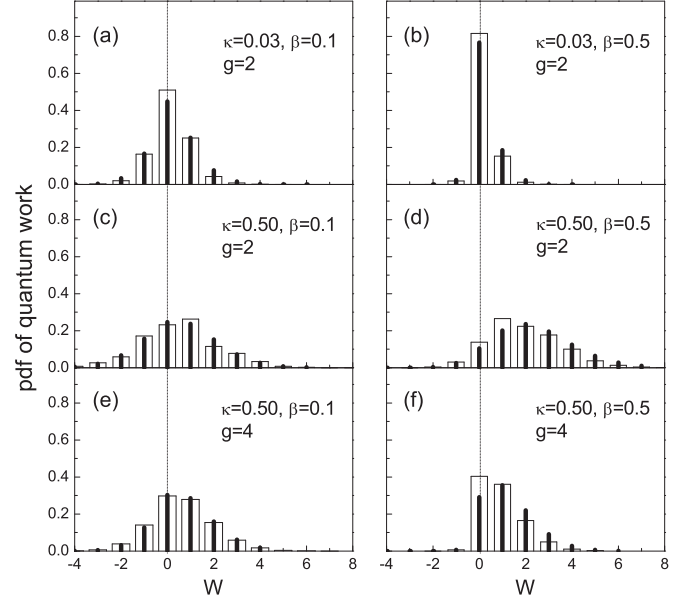

FIG. 2. The PDFs of the inclusive work for the TLS (37). The bars are calculated by simulating the quantum trajectories, while the solid bold lines are obtained by the CF method. The unit of work W is ω. In these panels the thin dashed lines at zero positions are guides for the eyes.

of these rates increase while their ratio is still unchanged. In this situation, not only does the population of trajectories with jumps become larger, but the frequency of the jumps in the same trajectory increases. Accordingly, the probability of zero work will considerably decrease while probabilities of the work with larger positive values are present. This is what we see in Fig. 2(d). The above arguments also imply that, if we prolong 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 negative work almost vanish. This is due to the fact that the larger field strength g leads to a negligible γ_+. Hence, the A_+ jumps that are responsible for the negative work are strongly inhibited. For the cases in the left column of the figure, analogous analyses can be performed. Because of the higher temperature (smaller β), 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 γ_+ and γ_- are comparable, which results in 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 work for adiabatic QMMEs. We have shown that this method is also useful in discussing the symmetry of the PDFs. Hence, the CF method provides us with an alternative way to study the quantum work besides the simulation of the quantum jump. The quantum master equations and the quantum jump theory were known to be complementary either in physical interpretations or in practical calculations. Our efforts here and before may be

thought of as concrete manifestations of this spirit about the theme of quantum work. Although the adiabatic quantum master equation and the equations that concern systems driven by weak fields are two often used time-dependent QMMEs, e.g., in the intriguing quantum heat engines [54], they do not definitely cover all situations. For instance, other master equations have been proposed for dissipative systems under intense and rapidly varying fields [55–59]. It will be interesting to investigate in future whether quantum work can be physically defined and what methods can effectively calculate it.

APPENDIX A: DERIVATIONS OF EQS. (24) AND (25)

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

$$E[W] = E[\varepsilon_\delta(t_f)] - E[\varepsilon_\alpha(0)] - \int_0^{t_f} \hbar\omega_{t_1} E[dN_+(t_1)] + \int_0^{t_f} \hbar\omega_{t_1} E[dN_-(t_1)]. \tag{A1}$$

On the basis of the relations [33]

$$E[\varepsilon_\delta(t)] = \text{Tr}[H(t)\rho(t)], \tag{A2}$$

$$E[dN_\pm(t)] = \gamma_\pm(\omega_t)\text{Tr}[A_\mp(t)A_\pm(t)\rho(t)]\, dt, \tag{A3}$$

Eq. (A1) can be rewritten as

$$\begin{aligned}E[W] &= \text{Tr}[H(t_f)\rho(t_f)] - \text{Tr}[H(0)\rho(0)] \\ &\quad + \int_0^{t_f} d\tau\, \hbar\omega_\tau \text{Tr}\{[\gamma_-(\omega_{t_1})A_+(t_1)A_-(t_1) \\ &\quad - \gamma_+(\omega_{t_1})A_-(t_1)A_+(t_1)]\rho(t_1)\} \\ &= \int_0^{t_f} dt_1 \frac{d}{dt_1}\text{Tr}[H(t_1)\rho(t_1)] \\ &\quad - \int_0^{t_f} dt_1 \text{Tr}[D_{t_1}^\star[H(t_1)]\rho(t_1)] \\ &= \int_0^{t_f} dt_1 \text{Tr}[\partial_{t_1} H(t_1)\rho(t_1)], \tag{A4}\end{aligned}$$

where $D_{t_1}^\star$ is the adjoint superoperator of D_{t_1} in Eq. (2). We see that the last two equations are just the *first law* of thermodynamics for the adiabatic quantum master equation (1) [41]. The derivation of Eq. (25) is more complicated. We first write

the explicit form of the left-hand side of the equation

$$\begin{aligned}E[W^2] &= E\{[\varepsilon_\delta(t_f) - \varepsilon_\alpha(0)]^2\} \\ &\quad + E\left[\left(\int_0^{t_f} dt_1 \hbar\omega_{t_1} dN_-(t_1)\right. \right. \\ &\quad \left.\left. - \int_0^{t_f} dt_2 \hbar\omega_{t_2} dN_+(t_2)\right)^2\right] \\ &\quad + 2E\left[[(\varepsilon_\delta(t_f) - \varepsilon_\alpha(0)])\left(\int_0^{t_f} dt_1 \hbar\omega_{t_1} dN_-(t_1)\right.\right. \\ &\quad \left.\left. - \int_0^{t_f} dt_2 \hbar\omega_{t_2} dN_+(t_2)\right)\right]. \tag{A5}\end{aligned}$$

In order to express these terms in the multiple time correlation functions of the operators, which now represent two time points, we need to exploit the following relations:

$$E[\varepsilon_\delta^2(t)] = \text{Tr}[H^2(t)\rho(t)], \tag{A6}$$

$$E[\varepsilon_\delta(t)\varepsilon_\alpha(0)] = \text{Tr}[H(t)G(t,0)H(0)\rho(0)], \tag{A7}$$

$$\begin{aligned}&E[\varepsilon_\delta(t_f)dN_\pm(t)] \\ &= \gamma_\pm(\omega_t)\text{Tr}[H(t_f)G(t_f,t)A_\pm(t)\rho(t)A_\mp(t)]dt, \tag{A8}\end{aligned}$$

$$\begin{aligned}&E[\varepsilon_\alpha(0)dN_\pm(t)] \\ &= \gamma_\pm(\omega_t)\text{Tr}[A_\mp(t)A_\pm(t)G(t,0)H(0)\rho(0)]\, dt. \tag{A9}\end{aligned}$$

The other three correlation functions concerning $E[dN_\pm(t_1)dN_\pm(t_2)]$ have been given in our previous study [30]. Substituting them in Eq. (A5) and doing 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 [30].

APPENDIX B: PROOF OF EQ. (35)

This relation between the propagator $\widetilde{\breve{G}}(s,0;\mu)$ and the adjoint propagator $\breve{G}^\star(t,t_f;-\nu)$ is a consequence of the characteristics of their generators,

$$\widetilde{\breve{\mathcal{L}}}_s(\mu)(O) = \Theta\breve{\mathcal{L}}_t^\star(-\nu)[\Theta^\dagger O\Theta]\Theta^\dagger. \tag{B1}$$

$\widetilde{\breve{\mathcal{L}}}_s(\mu)$ has been given in Eq. (31). We need to write out only one more:

$$\begin{aligned}\breve{\mathcal{L}}_t^\star(\mu)O &= \frac{i}{\hbar}[H(t),O] + \sum_{\alpha=\pm} \gamma_\alpha(\omega_t) \\ &\quad \times \left[e^{\alpha i\mu\hbar\omega_t} A_\alpha(t)O A_\alpha^\dagger(t) - \frac{1}{2}\{A_\alpha^\dagger(t)A_\alpha(t), O\}\right] \\ &\quad + \gamma_0\left[A_0(t)O A_0^\dagger(t) - \frac{1}{2}\{A_0^\dagger(t)A_0(t), O\}\right]. \tag{B2}\end{aligned}$$

Then the verification of Eq. (B1) is straightforward. Note that $\breve{\mathcal{L}}_t^\star(\mu)$ recovers the adjoint superoperator $\mathcal{L}_t^\star$ in Eq. (21) if μ is replaced by $-i\beta$.

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