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Quantum Jump Approach for Work and Dissipation in a Two-Level System

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We apply the quantum jump approach to address the statistics of work in a driven two-level system coupled to a heat bath. We demonstrate how this question can be analyzed by counting photons absorbed and emitted by the environment in repeated experiments. We find that the common nonequilibrium fluctuation relations are satisfied identically. The usual fluctuation-dissipation theorem for linear response applies for weak dissipation and/or weak drive. We point out qualitative differences between the classical and quantum regimes.

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The quantum jump (QJ) method, also called the Monte Carlo wave function technique, was developed in the early 1990s [1–4]. This development followed a series of experiments performed in the mid 1980s that reported the observation of QJs in ions [5–7], in conjunction with theoretical work concerning the nature of these jumps [8–10]. Subsequent experiments in quantum optics [11] have probed QJs associated with the birth and death of photons in a cavity. Averaging of many individual quantum trajectories is equivalent to solving the relevant master equation [3,12,13]. More recently, the QJ method has also been used to address issues related to measurements and entropy production in quantum systems [14–18].

In this Letter we propose to use the QJ method as an efficient means to discuss the problem of determining the statistics of work in driven quantum systems with dissipation, currently a topic of intense discussion [19,20]. In particular, unlike for classical systems [21,22], the full statistics of work and the resulting nonequilibrium fluctuation relations are still not well established for quantum systems. We approach the problem by constructing quantum trajectories based on the QJ method, and demonstrate the validity of nonequilibrium fluctuation relations in a driven two-level system (qubit) coupled to a dissipative environment. Using the same technique we discuss the two lowest moments of work in driven evolution. Figure 1 presents schematically the setup we consider. A two-level quantum system is driven by a classical source exerting work W on it. The system is also coupled to a thermal bath, with which it can exchange heat Q. The dynamics of the two-level system is determined by the combined action of the source and the environment.

We start by considering the driven two-level system in the absence of dissipation, described by the Hamiltonian

$$H_S = -\hbar\omega_0\sigma_z/2 + \lambda(t)(\sigma_+ + \sigma_-), \quad (1)$$

where σ_z is a Pauli matrix and $\sigma_+ = |e\rangle\langle g|$ and $\sigma_- = |g\rangle\langle e|$ are the raising and lowering operators in the ground $|g\rangle$–excited $|e\rangle$ state basis of the undriven system, $\hbar\omega_0 = E_e - E_g$ is the energy separation of the two levels, and $\lambda(t)$ is the drive signal of the source. A normalized quantum state $|\psi(t)\rangle$ describing this system at arbitrary time t can always be written as a superposition of the states $|g\rangle$ and $|e\rangle$: $|\psi(t)\rangle = a(t)|g\rangle + b(t)|e\rangle$ with $|a(t)|^2 + |b(t)|^2 = 1$. The infinitesimal time evolution of such a state is governed by the equation

$$|\psi(t+\Delta t)\rangle = [1 - i\Delta t H_S/\hbar]|\psi(t)\rangle, \quad (2)$$

which conserves the normalization.

Next consider the driven two-level system coupled to a bath with which it can exchange photons of frequency ω_μ. For definiteness, we assume the system-bath coupling Hamiltonian H_C to have the linear form

$$H_C = \sum_\mu c_\mu \sigma_+ b_\mu + c_\mu^* b_\mu^\dagger \sigma_-. \quad (3)$$

Suppose that at time t the total system is in a state

$$|\psi(t)\rangle = [a(t)|g\rangle + b(t)|e\rangle] \otimes |0\rangle; \quad (4)$$

i.e., the two-level system is in a generic superposition state, and the bath is in a state without any excess photons. At a slightly later time $t + \Delta t$ we have

$$|\psi(t+\Delta t)\rangle = |\psi^{(0)}(t+\Delta t)\rangle + |\psi^{(1)}(t+\Delta t)\rangle + |\psi^{(-1)}(t+\Delta t)\rangle, \quad (5)$$

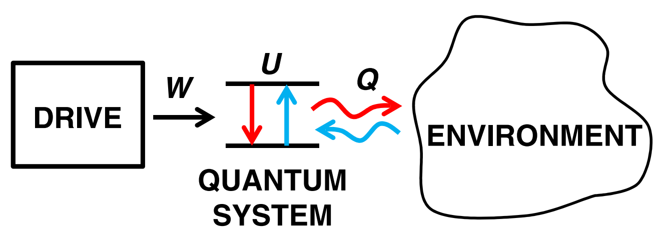

FIG. 1 (color online). A quantum two-level system (center) driven by an external force (left) and coupled to an environment (right).

where

$$|\psi^{(0)}(t+\Delta t)\rangle = [a(t+\Delta t)|g\rangle + b(t+\Delta t)|e\rangle] \otimes |0\rangle, \tag{6}$$

$$|\psi^{(1)}(t+\Delta t)\rangle = \sum_{\mu} \beta_{\mu,+}|g\rangle \otimes |n_\mu + 1\rangle, \tag{7}$$

$$|\psi^{(-1)}(t+\Delta t)\rangle = \sum_{\mu} \beta_{\mu,-}|e\rangle \otimes |n_\mu - 1\rangle. \tag{8}$$

We assumed Δt to be short enough that at most one photon is exchanged with the bath. The various components therefore involve only 0, 1, or -1 excess photons μ. The amplitudes $\beta_{\mu,\pm}$ can be obtained using standard time-dependent perturbation theory with respect to H_C; to the lowest order one finds [23]

$$\sum_{\mu} |\beta_{\mu,+}|^2 = |b(t)|^2 \Gamma_\downarrow \Delta t, \qquad \sum_{\mu} |\beta_{\mu,-}|^2 = |a(t)|^2 \Gamma_\uparrow \Delta t, \tag{9}$$

where

$$\Gamma_\downarrow = \frac{2\pi}{\hbar} \sum_{\mu} (n_\mu + 1)|c_\mu|^2 \delta(\hbar\omega_0 - \hbar\omega_\mu), \tag{10}$$

$$\Gamma_\uparrow = \frac{2\pi}{\hbar} \sum_{\mu} n_\mu |c_\mu|^2 \delta(\hbar\omega_0 - \hbar\omega_\mu) \tag{11}$$

are the photon emission and absorption rate, respectively. Here we assume that the time step Δt is short compared to the relevant time scale of the dynamics of the two-level system, yet long compared to the bath's correlation time so that energy conservation is accurate [24]. Note that $\Gamma_\uparrow/\Gamma_\downarrow = e^{-\beta\hbar\omega_0}$ (detailed balance), provided the bath remains in thermal equilibrium at all times, such that $n_\mu = (e^{\beta\hbar\omega_\mu} - 1)^{-1}$.

In order for $|\psi(t+\Delta t)\rangle$ [Eq. (5)] to be normalized, we have to impose $\langle\psi^{(0)}(t+\Delta t)|\psi^{(0)}(t+\Delta t)\rangle = 1 - \Delta p$, where

$$\Delta p = \Delta t[|a(t)|^2\Gamma_\uparrow + |b(t)|^2\Gamma_\downarrow]. \tag{12}$$

This can be achieved by modifying the standard time evolution into a non-Hermitian one, replacing in Eq. (2) the Hamiltonian H_S by

$$H = H_S - i\hbar\Gamma_\downarrow|e\rangle\langle e|/2 - i\hbar\Gamma_\uparrow|g\rangle\langle g|/2. \tag{13}$$

We are now in a position to define the QJ procedure. Let at time t the system be in the normalized state $|\psi(t)\rangle$. If no photon exchange occurs during the time interval Δt, it will be in a state

$$|\psi^{(0)}(t+\Delta t)\rangle = [1 - i\Delta t H/\hbar]|\psi(t)\rangle \tag{14}$$

at time $t+\Delta t$, with norm $1-\Delta p$. Hence the normalized state $|\psi(t+\Delta t)\rangle = |\psi^{(0)}(t+\Delta t)\rangle/\sqrt{1-\Delta p}$. Should a photon exchange (a QJ) occur during Δt, the normalized state will be either $|\psi(t+\Delta t)\rangle = |e\rangle$ or $|\psi(t+\Delta t)\rangle = |g\rangle$, depending on whether the photon was absorbed or emitted by the two-level system. The Monte Carlo procedure consists of choosing a random number ϵ between zero and one. If $\epsilon > \Delta p$, no QJ occurs, and we take $|\psi(t+\Delta t)\rangle = |\psi^{(0)}(t+\Delta t)\rangle/\sqrt{1-\Delta p}$. If $\epsilon < \Delta p$, a photon is either emitted with probability $|b(t)|^2\Gamma_\downarrow/[|a(t)|^2\Gamma_\uparrow + |b(t)|^2\Gamma_\downarrow]$ [state $|\psi(t+\Delta t)\rangle = |g\rangle$] or absorbed with probability $|a(t)|^2\Gamma_\uparrow/[|a(t)|^2\Gamma_\uparrow + |b(t)|^2\Gamma_\downarrow]$ [state $|\psi(t+\Delta t)\rangle = |e\rangle$]. It is easy to show (see the Supplemental Material [25]) that this procedure is equivalent to the analysis of the usual master equation for the partial density matrix, defined as the average of $|\psi(t)\rangle\langle\psi(t)|$ over the bath degrees of freedom [12,26]. Moreover, this procedure shows that the environment not only induces QJs, but also influences the evolution of the system in between such jumps, where the dynamics of the amplitudes a and b in the interaction representation is governed by

$$i\hbar\dot{a} = e^{-i\omega_0 t}\lambda(t)b + i\hbar\Delta\Gamma|b(t)|^2 a(t)/2, \tag{15}$$

$$i\hbar\dot{b} = e^{i\omega_0 t}\lambda(t)a - i\hbar\Delta\Gamma|a(t)|^2 b(t)/2 \tag{16}$$

with $\Delta\Gamma = \Gamma_\downarrow - \Gamma_\uparrow$.

Figure 2 is a numerical example of the evolution of the excited state population $|\langle e|\psi(t)\rangle|^2$, obtained using the QJ procedure. At times $t < 0$ the system is not driven, and it jumps between the two eigenstates $|e\rangle$ and $|g\rangle$ stochastically, governed by the rates $\Gamma_\downarrow$ and $\Gamma_\uparrow$, and the instantaneous populations. In the time interval $0 \le \omega_0 t/2\pi < 8$, the system is driven resonantly by the force $\lambda(t) = \lambda$. Within this interval, it makes one QJ down $|e\rangle \to |g\rangle$ in this particular realization. Finally, at times $\omega_0 t/2\pi \ge 8$, the drive is absent again, and the collapse (jump to $|e\rangle$) tells

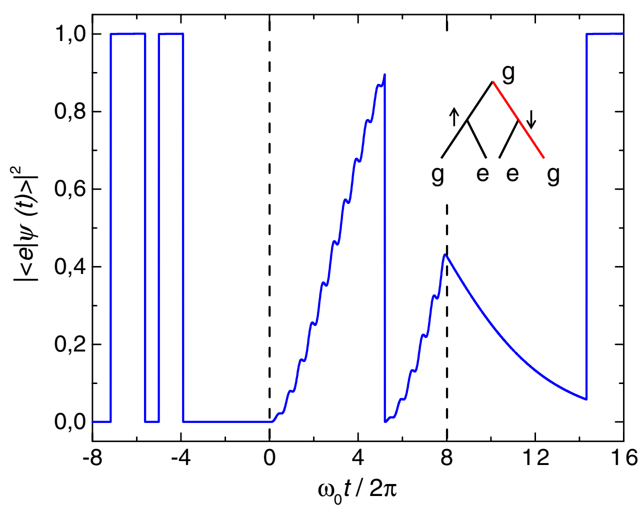

FIG. 2 (color online). An example of a quantum jump simulation. The environment temperature is $\beta\hbar\omega_0 = 1.0$. The amplitude of the harmonic drive (frequency $\omega = \omega_0$) is $\lambda_0 = 0.1\hbar\omega_0$ and lasts 8 cycles. The relaxation rate is given by $\Gamma_\downarrow = 0.1\omega_0$.

that the system was measured to be in the ground state at the end of the drive.

We next demonstrate that detecting the photons emitted and absorbed by calorimetry of the environment serves as a traditional projective measurement. Suppose that the system's wave function reads $|\psi(\mathcal{T})\rangle = a(\mathcal{T})|g\rangle + b(\mathcal{T})|e\rangle$ at the end of the driving period. The evolution of the amplitudes at times $t \geq \mathcal{T}$ is governed by Eqs. (15) and (16) with $\lambda = 0$, until the first "guardian" photon is exchanged. During this quiet period, the excited state population $p_e(t) = |b(t)|^2$ thus evolves as $\dot{p}_e = -\Delta\Gamma p_e(1 - p_e)$. Hence

$$p_e(t) = (1 + re^{\Delta\Gamma(t-\mathcal{T})})^{-1}, \tag{17}$$

where $r = [1 - p_e(\mathcal{T})]/p_e(\mathcal{T})$. We can then evaluate the probability P_E that the system is found to be in the excited state, indicated by the absorption of the guardian photon by the environment (as opposed to being emitted by the environment). Indeed,

$$P_E = \int_{\mathcal{T}}^{\infty} \Delta t \Gamma_{\downarrow} p_e(t) e^{-\int_{\mathcal{T}}^{t} \Delta t' [\Gamma_{\uparrow}(1-p_e(t')) + \Gamma_{\downarrow} p_e(t')]}, \tag{18}$$

and integrating Eq. (18) after substitution of $p_e(t)$ from Eq. (17) yields $P_E = p_e(\mathcal{T})$. This intuitive result holds irrespective of the values of $\Gamma_{\uparrow}$ and $\Gamma_{\downarrow}$; i.e., it is valid at any temperature of the environment and independent of the strength and type of the coupling. This is in accordance with the result of a projective measurement of the state of a quantum system.

Based on the interpretation of traces as that in Fig. 2, we obtain the work for a given realization as follows. We make two measurements, in the spirit of the two-measurement protocol that was formerly applied to an isolated driven system [20,27]: one measurement before the driving period, and another one after it. These measurements are done by the detection of the last photon emitted to the environment or absorbed by the system to the environment before the drive and of the first photon after the drive. This can be realized in practice calorimetrically as proposed in Ref. [28]. In the example of Fig. 2, (i) the first measurement indicates that the initial state of the system is $|g\rangle$ (internal energy $U_i = E_g$), since the last photon before the application of the force (at $\omega_0 t/2\pi \simeq -4$) was emission by the system, and (ii) the second measurement shows that the final state of the system was likewise $|g\rangle$ (internal energy is $U_f = E_g$), since the first photon after the drive (at $\omega_0 t/2\pi \simeq 14$) was absorption by the system. These two measurements thus tell that the force has not changed the system internal energy U, i.e., $\Delta U = U_f - U_i = 0$ for this particular realization. (The other possible outcomes would have been $\Delta U = \pm\hbar\omega_0$.) During the drive, heat is released to or taken from the environment by the QJ events. Again, in the example of Fig. 2, the one photon emitted by the system corresponds to assigning heat $Q = +\hbar\omega_0$ released to the environment. The work done by the source is then $W = \Delta U + Q$, and equals $\hbar\omega_0$ for this realization. Our ultimate task is then to find the distribution of W in repeated experiments, and to assess the fluctuation relations and the various moments of W.

We proceed by presenting a systematic method to analyze the statistics of work and heat under the force protocol $\lambda(t)$ from the initial time 0 to the final time $\mathcal{T}$. At time $t = 0$, the system is supposed to be equilibrated by the heat bath. As a result it will occupy the ground state with probability $p_g = (1 + e^{-\beta\hbar\omega_0})^{-1}$ and the excited state with probability $p_e = e^{-\beta\hbar\omega_0} p_g$. Therefore, to obtain averages involving W under many repetitions of the protocol $\lambda(t)$, two cases should be distinguished. One corresponds to the case where the protocol is run on the ground state, the other to the case where the protocol is run on the excited state. For both cases, the set of possible quantum trajectories can be represented with the help of a Cayley tree. The inset of Fig. 2 shows the Cayley tree corresponding to all possible quantum trajectories starting from the ground state and undergoing one QJ during the driving period $\mathcal{T}$. Specifically, the trajectory in red is the one realized during the simulation shown in Fig. 2. The probability P for such a single photon trajectory starting in the ground state is given by

$$P = p_g \Gamma_{\downarrow} \int_0^{\mathcal{T}} dt |a_g(\mathcal{T}, t)|^2 e^{-\pi_g(\mathcal{T}, t)} |b_g(t, 0)|^2 e^{-\pi_g(t,0)}. \tag{19}$$

Here $b_g(t, 0)$ denotes the probability amplitude b at time t with the ground state $b(0) = 0$ as the initial condition at $t = 0$. Similarly, $a_g(\mathcal{T}, t)$ denotes the probability amplitude a at time $\mathcal{T}$ with the ground state $a(t) = 1$ as the initial condition at time t. Here a and b are found by solving Eqs. (15) and (16). The probability that no photon is exchanged with the bath is given by the Poisson factor $e^{-\pi_g}$, where we defined

$$\pi_{g,e}(t_2, t_1) = \int_{t_1}^{t_2} dt [\Gamma_{\uparrow} |a_{g,e}(t, t_1)|^2 + \Gamma_{\downarrow} |b_{g,e}(t, t_1)|^2]. \tag{20}$$

The total probability P_1 for a one-photon process to occur under the action of the drive is found by summing over all trajectories for this tree and for the one corresponding to the initial excited state.

The calculation of averages involving the quantity W is now immediate. For example, along the trajectory analyzed above we have $W = \hbar\omega_0$. This trajectory thus contributes to $\langle W^k \rangle$ as $(\hbar\omega_0)^k P/P_1$ and to $\langle e^{-\beta W} \rangle$ as $e^{-\beta\hbar\omega_0} P/P_1$. The other trajectories can be analyzed similarly; the extension to Cayley trees corresponding to arbitrary n-photon processes is straightforward. In Fig. 3 we show the results of calculations of the ratio of the two lowest moments of W as well as of the quantity $\langle e^{-\beta W} \rangle$. The points are obtained with QJ simulations; the solid lines correspond to a perturbative solution of Eqs. (15) and (16) for weak dissipation

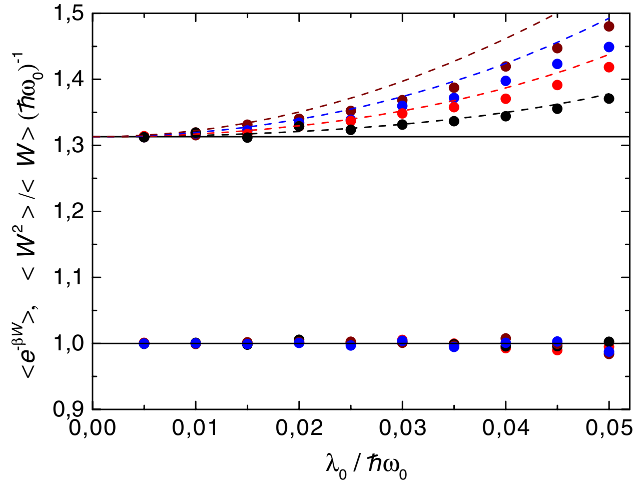

FIG. 3 (color online). Results of numerical simulations and analytic approximations. The ratio of the two lowest moments of work and the JE average are shown as functions of the driving amplitude. The symbols are numerical simulations and the lines are analytical approximations; the colored ones are for the perturbative in $\Gamma_{\downarrow,\uparrow}$ calculation. Here, $\beta\hbar\omega_0 = 2.0$, the resonant ($\omega = \omega_0$) drive lasts 10 cycles, and the various data sets are for $\Gamma_\downarrow = (0,)0.005, 0.01, 0.015, 0.02$ from bottom to top.

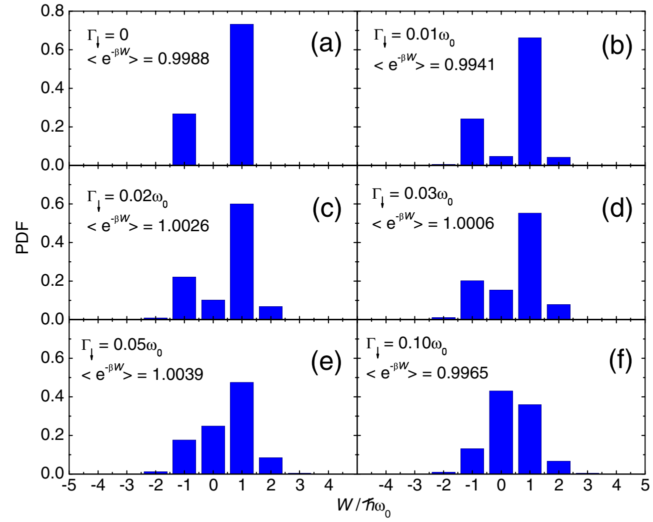

FIG. 4 (color online). Numerically calculated work distributions under the influence of the π pulse. The system, initially in thermal equilibrium, is driven at the resonance angular frequency ω_0 over 10 periods, with amplitude $\lambda_0 = 0.05\hbar\omega_0$. The bath temperature is given by $\beta\hbar\omega_0 = 1$, and we employed 10^5 repetitions for each value of $\Gamma_\downarrow$. Panel (a) presents an isolated qubit, whereas panels (b)–(f) correspond to open systems with increasing relaxation.

(see the Supplemental Material [25]). In the linear response limit $\lambda_0 \to 0$, we find that the ratio $\langle W^2\rangle/\hbar\omega_0\langle W\rangle \to \coth(\beta\hbar\omega_0/2) \simeq 1.31$, the usual fluctuation-dissipation result. As λ_0 is increased, deviations are found from linear response that are more important for stronger dissipation; perturbation theory breaks down at relatively low drive amplitudes.

We now turn to the results for the quantity $\langle e^{-\beta W}\rangle$. The simulations show that within the numerical accuracy this quantity equals 1 for the parameter range studied here, in agreement with the celebrated Jarzynski equality (JE) $\langle e^{-\beta W}\rangle = 1$ [21,29]. (Since the drive lasts over an integer number of periods, the free-energy difference between the initial and final points vanishes, and the right-hand side of this equation is indeed expected to be equal to unity.) Analyzing the Cayley tree trajectories systematically, one can demonstrate the validity of the JE for the dissipative driven two-level system studied here (see the Supplemental Material [25]). The proof is based on the fact that the quantity $\langle e^{-\beta W}\rangle$ is equal to the (normalized) total probability for all the trajectories under the reverse protocol $\lambda_R(t) = \lambda(\mathcal{T} - t)$, provided the rates $\Gamma_\uparrow$, $\Gamma_\downarrow$, as well as the probabilities p_e and p_g, satisfy detailed balance. We like to emphasize that on one hand this proof, based on reversed trajectories, is analogous to the early one by Crooks for a classical two-state system obeying detailed balance for transition rates [30]. Yet the classical dynamics, presenting definite alternating transitions between the two states, differs from the quantum evolution involving superposition states, leading to the branching of the trajectories shown by the Cayley trees.

A two-level system driven sinusoidally over a time $\mathcal{T} = \pi/\lambda_0$ at angular frequency ω_0 undergoes a so-called π pulse, ending up into the excited state if it was initially in the ground state, and vice versa. Figure 4 shows the corresponding work distribution calculated for various rates of relaxation. Initially the system is in thermal equilibrium. Figure 4(a) shows the probability distribution function for vanishing relaxation rate. In this case the work has two possible values: $-\hbar\omega_0$ with probability p_e, and $+\hbar\omega_0$ with probability p_g. Upon increasing the relaxation rate in Figs. 4(b)–4(d) and 4(f), the probability distribution function evolves from the "bimodal" one into a more bell-shaped distribution. For all values of relaxation, the JE is satisfied within the numerical error; the values obtained by 10^5 repetitions in each case are indicated in the corresponding panel.

A natural realization of the presented scheme is a superconducting phase qubit [31,32] coupled inductively to a dissipative element, whose temperature can be monitored in real time in order to perform a calorimetric measurement [28]. Specifically, one may use a current-biased SQUID, yielding a two-level system with a typical level spacing of the order of $\hbar\omega_0/k_B \sim 1$ K. The rates are given by $\Gamma_\downarrow = g^2 S(+\omega_0)$ and $\Gamma_\uparrow = g^2 S(-\omega_0)$. The coupling g is proportional to the mutual inductance between the SQUID loop and the dissipative element; i.e., it is determined by the geometry of the setup. The noise spectral function $S(\pm\omega_0)$ of the resistive element is taken at angular frequency $\pm\omega_0$. For thermal noise, detailed balance between the $\downarrow, \uparrow$ rates is obeyed.

In summary, we have analyzed work in a disipative two-level quantum system using the quantum jump approach. The common fluctuation theorem (JE) is shown to be valid, and we obtain the moments of work distribution in linear response and beyond. As an illustration, we apply the method to a qubit driven by a π pulse and we demonstrate that the model can be realized for instance as a superconducting phase qubit.

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[24] The numerical results presented in this Letter have been obtained for $\omega_0 \Delta t = 2\pi/100$. We explicitly checked that an increase of this parameter up to $\omega_0 \Delta t = 2\pi/3$ does not alter the results significantly.
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