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Work and its fluctuations in a driven quantum system

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We analyze work done on a quantum system driven by a control field. The average work depends on the whole dynamics of the system, and is obtained as the integral of the average power operator. As a specific example we focus on a superconducting Cooper-pair box forming a two-level system. We obtain expressions for the average work and work distribution in a closed system, and discuss control field and environment contributions to the average work for an open system.

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The fluctuation relations (FRs)1,2 govern work and dissipation in small classical systems when they are driven out of equilibrium. They have recently attracted much attention because of their applications in molecular systems.3 Fluctuation relations can also be accurately studied in single-electron transport.4–6 A natural question is if similar concepts and experiments can be extended to the quantum regime. The first attempts in this direction focused on finding a proper work operator.1,7–10 However, after a long debate, it has become clear that this approach has serious drawbacks.11 Work is defined through a two-measurement process (TMP).10–16 The energy of the system is determined by the corresponding energy difference. This definition has the advantage that the work done in a process is determined by the corresponding energy difference. It is recovered if the system is initially in an eigenstate or in a superposition of the eigenstates of \( \hat{H} \). Fluctuation relations on the right-hand side are given by the unitary and dissipative dynamics, respectively. By substituting the above result into Eq. (2), we find that there is no contribution due to the unitary dynamics since \( \text{Tr}[\{\hat{H}, \hat{\rho}\}] \) vanishes. Then the average power reads

\[
\langle \hat{P}(t) \rangle = \frac{d}{dt} \langle \hat{H} \rangle = \text{Tr} \left\{ \frac{d\hat{\rho}}{dt} \hat{H} \right\} + \langle \hat{P} \rangle.
\]

Under quite general assumptions the dynamics of the reduced density operator of the system can be described by a master equation19

\[
d\hat{\rho}/dt = -\frac{i}{\hbar} [\hat{H}, \hat{\rho}] + \hat{L}(\rho),
\]

where the contributions on the right-hand side are given by the unitary and dissipative dynamics, respectively. 

The average work definition in Eq. (3) is more general than the TMP since it takes into account the full quantum evolution.

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Cooper-pair box as a driven quantum two-level system. We consider a Cooper-pair box (CPB) consisting of a superconducting island connected to a superconducting lead by a Josephson tunnel junction. The system is described by the circuit scheme in the inset in Fig. 2 and it is characterized by a voltage source \( V_{x} \), coupling capacitance \( C_{g} \), a Josephson junction with energy \( E_{J} \), and capacitance \( C_{J} \). We denote \( C_{\Sigma} \equiv C_{g} + C_{J} \). Resistor \( R \) to be discussed in the last part of this Rapid Communication, forms the dissipative environment of the box. This system is a candidate for a calorimetric measurement of quantum work distribution.\(^{25}\)

In the regime \( \epsilon \equiv E_{J}/(2C_{\Sigma}) \ll 1 \), where \( C_{\Sigma} = 2C_{g}^{2}/C_{g} \) is the charging energy of the box, we can treat the CPB as a two-level quantum system. Denoting with \( |0\rangle \) and \( |1\rangle \) the state with zero and one excess Cooper pair on the island, respectively, the Hamiltonian reads

\[
\hat{H} = -E_{C}q(|1\rangle\langle 1| - |0\rangle\langle 0|) - \frac{E_{J}}{2}(|1\rangle\langle 0| + |0\rangle\langle 1|),
\]

where \( q = C_{g}V_{x}/(2e) - 1/2 \) is the normalized gate voltage. We assume driven evolution: a linear gate ramp \( q(t) = -1/2 + t/T \) over a period \( T \) starting from \( t = 0 \). The ground and the excited states of the system are separated by the energy gap \( \hbar\omega_{0} = 2E_{C}\sqrt{q^{2} + e^{2}} \) which reaches the minimum \( E_{J} \) at \( t = T/2 \) (see Fig. 1). We recover the standard Landau-Zener (LZ) model\(^{26,27}\), where the system is excited when driven in a nonadiabatic way through a avoided crossing.

The time-dependent eigenstates of the Hamiltonian (4) are \( |g\rangle = \frac{1}{\sqrt{2}}(|\sqrt{1-\eta}|\langle 0| + \sqrt{1+\eta}|1\rangle\langle 1|) \) and \( |e\rangle = \frac{1}{\sqrt{2}}(\sqrt{1+\eta}|0\rangle - \sqrt{1-\eta}|1\rangle\langle 1|) \), where \( \eta = q/\sqrt{q^{2} + e^{2}} \).\(^{28}\)

For this system, the power operator is \( \hat{P} = E_{C}q(1-2\eta) \), where \( \eta = |\langle 1|\rangle \) is the operator of the number of Cooper pairs on the island and \( \mathbb{I} = |1\rangle\langle 1| + |0\rangle\langle 0| \) is the identity operator. We calculate the time-dependent average of the power operator in the Heisenberg picture, \( \hat{P}^{H}(t) = U(t)^{\dagger}\hat{P}U(t) \), with the time evolution operator \( U(t) \), and the state \( |\psi(0)\rangle \) that does not change in time. Here we focus on the first and second moments of the work done on the CPB, which can be expressed through \( \hat{P}^{H}(t) \) as \( \langle W \rangle = \int_{0}^{T} dt \langle \hat{P}^{H}(t) \rangle \) and \( \langle W^{2} \rangle = \int_{0}^{T} dt_{1} \int_{0}^{T} dt_{2} \langle \hat{P}^{H}(t_{2})\hat{P}^{H}(t_{1}) \rangle \), where \( \langle \cdot \cdot \rangle \equiv \langle \psi(0)| \cdot |\psi(0)\rangle \). Explicitly,

\[
\langle W \rangle = E_{C}\left(1 - \frac{2}{T^{2}}\int_{0}^{T} \langle \hat{H}^{H}(t) \rangle dt \right)
\]

and

\[
\langle W^{2} \rangle = 2E_{C}\langle W \rangle - E_{C}^{2}\left[1 - \frac{4}{T^{2}}\int_{0}^{T} dt_{1} dt_{2} \int_{0}^{T} \langle \hat{H}^{H}(t_{2})\hat{H}^{H}(t_{1}) \rangle \right].
\]

Equations (5) and (6) can be applied for both closed and open systems.\(^{19,29,30}\)

**Instantaneous transition regime, unitary evolution.** If the time of the control ramp is much shorter than the relaxation and dephasing times, the evolution of the system can be considered unitary. For \( \epsilon \ll 1 \), the LZ transitions are localized near the minimum energy gap at \( t = T/2 \) and the dynamics is well approximated by the instantaneous transition model\(^{31,32}\), i.e., the evolution is composed of pure adiabatic evolution and instantaneous LZ transitions at \( t = T/2 \) (see Fig. 1). All work, spent exactly in these LZ transitions, is stored in the system (CPB) as increased internal energy. Along the adiabatic region, the evolution operator reads \( U(t) = \exp \left[-i\hat{H}_{0}t/\hbar \right] \). This difference is highlighted in Fig. 2(a), where we plot the analytical result \( \langle g(T/2)\rangle \) and the state \( |\psi(T/2)\rangle \) for different initial states. The oscillatory behavior of \( \langle g(T/2)\rangle \) for different initial states. The oscillating behavior of \( \langle g(T/2)\rangle \) is a function of \( \Gamma \). The first term represents the work done on the system which is initialized in the ground or in the excited state, i.e., \( \alpha = 1 \) or 0, respectively. The second term with its characteristic oscillatory behavior is due to the quantum interference at the LZ avoided crossing.\(^{32}\) This additional contribution is always present when the system is initially in a coherent state and it is a clear difference with the respect to the TMP. This difference is highlighted in Fig. 2(a), where we plot the analytical result in Eq. (8) as a function of \( T \) for different initial states. The oscillating behavior of \( \langle W \rangle \) is obtained for \( \alpha = 1/\sqrt{2} \) and \( \gamma = 0 \) and we should compare it with the prediction of the TMP \( \langle W \rangle = 0 \). The two exponential decays with \( P_{LZ} \) are obtained for the ground and excited initial states, \( \alpha = 1 \) and \( \alpha = 0 \) with...
and the system initialized in the ground state, this equation gives $G(u) = 1 + P_{LZ}(e^{iuE_C} - 1)$, which corresponds to the following work distribution:

$$\rho(W) = (1 - P_{LZ})\delta(W) + P_{LZ}\delta(W - E_C). \quad (9)$$

This distribution agrees with the first two moments and can be used to find the higher moments.

**Open system with slow and fast relaxation.** The most interesting and nontrivial test of Eq. (3) is when the system interacts with the environment during the evolution of $q$. To evaluate the heat contribution in Eq. (3) we need to consider a concrete example of the system-environment interaction. If the time and the ramp time are of the same order, dissipation $Q$ takes place during the driven evolution. To evaluate dissipation during the sweep, we then solve the master equation (ME) of the CPB adapted from the corresponding ME of Refs. 28 and 34. This ME and some details of the analysis are given in the SM. The environment is described by the resistor $R$ coupled capacitively to the island of the CPB (inset in Fig. 2).

As above, we assume that the temperature is low as compared to the excitation energy. If the system is initially in the ground state, the average heat released to the environment during the ramp normalized by the total work done for a few values of $\epsilon$ is shown in Fig. 3(a) based on the numerical solution of the

In this specific case, the first two moments of work calculated above agree with the full work distribution $\rho(W)$ which for a closed system with unitary evolution $U(T)$ can be found essentially by direct comparison of the initial, $H(0)$, and final, $H(T)$, Hamiltonian of the system. Indeed, the work generating function $G(u)$ (Fourier transform of the distribution) can be written as (see, e.g., Ref. 11) $G(u) = \text{Tr}[U(T)e^{iuH(T)}U(T)^{-1}e^{-iuH(0)}\rho_0]$, where $\rho_0$ is the initial density matrix of the system assumed to be diagonal together with the initial Hamiltonian $H(0)$. For the CPB considered above

FIG. 2. (Color online) (a) Average work $\langle W \rangle$ normalized to $E_C$ for different initial states: $\alpha = 1/\sqrt{2}$ and $\gamma = 0$ (blue oscillating curve), ground state $\alpha = 1$ and $\gamma = 0$ (top black exponentially decaying curve), and excited state $\alpha = 0$ and $\gamma = 0$ (lower black exponentially decaying curve). The purple curve denotes the behavior $\sqrt{P_{LZ}(1 - P_{LZ})}$. (b) Work variance $\langle \delta W^2 \rangle$ normalized to $E_C^2$. The blue solid lines contain the oscillatory behavior for initial state $\alpha = 1/\sqrt{2}$ and $\gamma = 0$. The black dashed line is obtained for the initial state, $\alpha = 1$ and $\gamma = 0$ (ground state). We have used $\epsilon = E_J/(2E_C) = 0.05$. Inset: Circuit scheme of the Cooper-pair box (CPB) connected to a dissipative environment $R$.

$\gamma = 0$, respectively. The behavior for the thermalized initial density matrix can be obtained from these two curves with the correct weighted average.

With the same approach, the evaluation of Eq. (6) yields $\langle W^2 \rangle = P_{LZ}E_C^2$ for the second moment, independent of the initial state. With these results the corresponding rms fluctuation of work can be immediately calculated as $\langle \delta W^2 \rangle = \langle W^2 \rangle - \langle W \rangle^2$. Figure 2(b) shows the behavior of $\langle \delta W^2 \rangle$ for different initial states. Numerical simulations confirm the analytical results presented in Fig. 2.

The definition of work in Eq. (3) and the TMP give the same results if the system is initially in an eigenstate of $H(0)$ or an incoherent superposition of them. In the interesting case in which the system is initialized in the ground state, i.e., $\alpha = 1$, and for nearly adiabatic drive ($P_{LZ} \ll 1$), we have a linear response result linking the average work and its fluctuations as $\langle \delta W^2 \rangle = E_C\langle W \rangle$.

FIG. 3. (Color online) (a) Numerically calculated (solid lines) dissipated average heat during the sweep in an open CPB as a function of the sweep time when the system is initially in the ground state. The system-environment coupling constant is chosen to be $C_g/C_X = 0.05$ here, $E_C/k_B = 1$ K, and the environment resistance is $R = 1 \times 10^4$ $\Omega$. The different curves from top to bottom correspond to $\epsilon = 0.05, 0.0375$, and 0.025. The dashed line is the analytic approximation of Eq. (10). (b) Dissipated average heat at $E_C T/h = 150, 100$, and 50 from top to bottom as a function of $\epsilon^2$. The other parameters and the line conventions are as in (a).
The integrand in the heat contribution in Eq. (3) can be conveniently written as \(-\hbar \rho_{gg}\omega_0\). If we denote with \(\Gamma_{gg}\) and \(\Gamma_{ge}\) the excitation and relaxation rates, respectively, in the semiclassical limit we have \(\rho_{gg} = -\Gamma_{gg}\rho_{gg} + \Gamma_{ge}\), where \(\Gamma_{ge} = \Gamma_{gg} + \Gamma_{ge}\), \(\Gamma_{gg}/\Gamma_{ge} = \exp(-\beta\omega_0\omega_0)\), and \(\beta\) is the inverse temperature of the environment. We use the trial solutions \(\rho_{gg} = \rho_{gg}^{(0)} + \delta\rho_{gg}^{(1)}\), where \(\rho_{gg}^{(0)} = \Gamma_{ge}/\Gamma_{ge}^{(0)}\) is the stationary solution and \(\delta\rho_{gg}^{(1)}\) is the correction due to the drive. Plugging \(\rho_{gg}\) in the initial equation we obtain \(\delta\rho_{gg}^{(1)} = -\rho_{gg}^{(0)}/\Gamma_{gg}\). When integrated the adiabatic contribution \(\hbar \rho_{gg}^{(0)}\omega_0\) gives no contribution (see SM33) and, with an integration by parts, the nonvanishing contribution in the limit \(\beta\, E_C \gg 1\) can be written as

\[
Q = \frac{4E_C^2}{hT} \int_{-\frac{1}{2}}^{\frac{1}{2}} dq \frac{q}{\omega_0}\frac{d}{dq} \left( \frac{\Gamma_{gg}}{\Gamma_{ge}} \right) = \frac{\beta E_C^2}{T} \int_{-\frac{1}{2}}^{\frac{1}{2}} dq \frac{\eta^2}{\Gamma_{ce} \cosh^2 \left( \frac{\omega_0}{2} \right)}.
\]

Here the second line arises from the detailed balance of the transition rates. Thus, we recover the expected properties of the released heat: (i) it depends on the full evolution which, in this limit, is represented by the driving parameter \(q\), (ii) it scales as \(1/T\), and (iii) it is positive.35

In summary, we have analyzed work done by a driving field on a quantum system. The obtained expression of average work has a physical interpretation, allowing one to assign separate contributions to the change in the internal energy and the heat dissipated to the environment in the spirit of the first law of thermodynamics. We applied our results to a two-level system, obeying in the first case unitary evolution and then in the presence of weak dissipation. For an open system, we presented a detailed analysis of the released heat two regimes where the relaxation time was either of the order or smaller than the driving time. In the latter case, our approach allows an analytical calculation of the released heat which has and immediate physical interpretation.

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