Statistics of work performed on a forced quantum oscillator

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Various aspects of the statistics of work performed by an external classical force on a quantum mechanical system are elucidated for a driven harmonic oscillator. In this special case two parameters are introduced that are sufficient to completely characterize the force protocol. Explicit results for the characteristic function of work and the corresponding probability distribution are provided and discussed for three different types of initial states of the oscillator: microcanonical, canonical, and coherent states. Depending on the choice of the initial state the probability distributions of the performed work may greatly differ. This result in particular also holds true for identical force protocols. General fluctuation and work theorems holding for microcanonical and canonical initial states are confirmed.

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I. INTRODUCTION

During the last decade various fluctuation and work theorems [1,2] have been formulated and discussed. They characterize among other things the full nonlinear response of a system under the action of a time-dependent force [3,4]. These theorems have been derived and experimentally confirmed primarily for classical systems [5-7]. Quantum mechanical generalizations were proposed recently [8-15].

Conceptual problems arise, though, in the context of quantum mechanics if one tries to generalize those classical relations that require, for example, the specification of a system's trajectory extending over some interval of time, or the simultaneous measurement of noncommuting observables. For example, the measurement of work performed by an external force on an otherwise isolated system may be accomplished in the framework of classical physics in principle in two different ways. The first method is based on two measurements of the energy, one at the beginning and the second at the end of the considered process. This method becomes unreliable in practice if the system is large and the work performed on the system is negligibly small compared to the total energy of the system. Such a situation typically arises if the system of interest, on which the force exclusively acts, interacts with its environment. In order to retain an isolated system, the large system made of the open system and its environment must be considered. Again, the work performed on the system results as the difference of the energies of the total system, which may both be very large.

For classical systems, this unfortunate situation can be circumvented by a second method, by monitoring the state of the relevant small system during the time when the force is acting. Having this information at hand, one can determine the work by integrating the power supplied to the system at each instant of time. The respective power can be inferred from the registered state of the system and the known force protocol. In a quantum system, a continuous measurement of even a single observable would strongly influence and possibly manifestly distort the system's dynamics. Clearly, only the first of the two methods of energy measurement is feasible, at least in principle, in the quantum context.

An alternative method based on continuous monitoring has recently been suggested by Esposito and Mukamel [11]

for open quantum systems described by Markovian quantum master equations. There the dynamics of the density matrix is mapped onto a classical rate process for which known fluctuation theorems can be applied [16]. This provides an interesting formal approach but its physical meaning has remained unclear [11]. Moreover, this approach is restricted to open systems that only weakly interact with their respective environments.

In the present paper, the distribution of work is discussed for the exactly solvable system of a driven harmonic oscillator [15,17]. In this case, the distribution of work is discrete. We provide formal expressions for this distribution and its corresponding characteristic function which are valid for all initial states of the system as well as for all possible kinds of force protocols. In particular, we determine the characteristic functions and distributions of the work for microcanonical, canonical, and coherent initial states which lead to qualitatively different work distributions.

The paper is organized as follows. In Sec. II we review the general form of the characteristic function of work performed on a system in terms of a correlation function of the exponentiated Hamiltonians at the initial and final times of the force protocol. We prove that this particular expression indeed always represents a characteristic function, i.e., the Fourier transform of a probability density. Section III presents various fluctuation and work theorems for canonical and microcanonical initial states. In Sec. IV general expressions for the characteristic function and the corresponding probability distribution of work are derived for a driven harmonic oscillator. Moreover, the expressions for the first four cumulants are derived. The dependence of the work distribution on the force protocol for microcanonical, canonical, and coherent initial states as well as its dependence on the specific parameters of these initial states are investigated.

II. CHARACTERISTIC FUNCTION OF WORK

The response of a quantum system on a perturbation by a classical, external force can be characterized by the change of energies contained in the total system. The energy as an observable coincides with the Hamiltonian H(t) of the total system. It includes the external force and therefore depends

on time. We will consider the dynamics of the system only within a finite window of time $[t_0, t_f]$ during which the force is acting in a prescribed way, resulting in a protocol of Hamiltonians which is denoted by $\{H(t)\}_{t_f,t_0}$. Apart from the action of the external force the system is assumed to be closed. Its dynamics is consequently governed by a unitary time evolution U_{t,t_0} , which is the solution of the Schrödinger equation

$$i\hbar \partial U_{t,t_0}/\partial t = H(t)U_{t,t_0}, \quad U_{t_0,t_0} = 1.$$
 (1)

As explained in the Introduction, the work *w* is measured as the difference between the energies of the system at the final and initial times t_f and t_0 . In a single measurement the work is given by the difference of two eigenvalues $e_n(t_f)$ and $e_m(t_0)$ of the Hamiltonians H(t) at the respective times t_f and t_0 , i.e., by $w = e_n(t_f) - e_m(t_0)$. The inherent randomness of the outcome of a quantum measurement in general leads to a measured work that is random. A complete description of the statistical properties of the work performed on the system is provided by the characteristic function $G_{t_f,t_0}(u)$ which presents the Fourier transform of the probability density of the work $p_{t_f,t_0}(w)$, i.e.,

$$G_{t_{f},t_{0}}(u) = \int dw \ e^{iuw} p_{t_{f},t_{0}}(w).$$
(2)

It can be expressed as a quantum correlation function of the exponentiated Hamiltonian at the initial and the final times [14], i.e.,

$$G_{t_{f},t_{0}}(u) = \langle e^{iuH(t_{f})}e^{-iuH(t_{0})} \rangle \equiv \text{Tr} \ e^{iuH_{H}(t_{f})}e^{-iuH(t_{0})}\overline{\rho}(t_{0}), \quad (3)$$

where

$$H_{H}(t_{f}) = U_{t_{f},t_{0}}^{\dagger}H(t_{f})U_{t_{f},t_{0}}$$
(4)

denotes the Hamiltonian in the Heisenberg picture. The density matrix $\bar{\rho}(t_0)$ follows from the initial density matrix $\rho(t_0)$ as a result of the measurement of the Hamiltonian $H(t_0)$. It is given by

$$\bar{\rho}(t_0) = \sum_n P_n(t_0)\rho(t_0)P_n(t_0),$$
(5)

where the operators $P_n(t_0)$ denote the eigenprojection operators of the Hamiltonian at time t_0 , which present a partition of unity:

$$\sum_{n} P_{n}(t_{0}) = 1.$$
 (6)

Before we apply the general expression (3) to a particular system and investigate its dependence on the initial state $\rho(t_0)$, we discuss three general properties of the correlation expression (3) which guarantee that the resulting function $G_{t_f,t_0}(u)$ indeed always presents a proper characteristic function of a classical random variable w.

(i) $G_{t_p t_0}(u)$ is a continuous function of u.

(ii) $G_{t_{f}t_{0}}(u)$ is a positive definite function of u, i.e., for all integer numbers n, all real sequences $u_{1}, u_{2}, \ldots, u_{n}$, and all complex numbers z_{i} , $i=1,2,\ldots,n$,

$$\sum_{i,i'}^{n} G_{t_{j},t_{0}}(u_{i} - u_{i'})z_{i}^{*}z_{i'} \ge 0$$
(7)

holds. Here, the asterisk z_i^* denotes the complex conjugate of z_i .

(iii) $G_{t_{e},t_{0}}(0) = 1.$

According to a theorem by Bochner [18] the properties (i)–(iii) are necessary and sufficient conditions for the function $G_{t_{f},t_0}(u)$ to be the Fourier transform of the probability measure of a random variable. In short, the first condition ensures that, strictly speaking, the function $G_{t_{f},t_0}(u)$ is the Fourier transform of a measure, the second condition assures that this measure is positive, and the third condition that it is normalized. Hence the correlation expression Eq. (3) always defines a proper characteristic function. A proof of the properties (i)–(iii) can be found in Appendix A.

III. CANONICAL AND MICROCANONICAL INITIAL STATES

In experiments an external force is often applied on a system that initially is found in a thermodynamic equilibrium state. Depending on whether the system was in weak contact with a heat bath or was totally isolated from its environment, the initial state of the system is described by either a canonical or a microcanonical density matrix. For both situations fluctuation and work theorems are known. We will briefly review these relations.

A. Work and fluctuation theorems for canonical initial states

If the initial density matrix is canonical, i.e., if

$$\rho(t_0) = Z^{-1}(t_0) \exp[-\beta H(t_0)], \qquad (8)$$

where

$$Z(t_0) = \text{Tr} \exp[-\beta H(t_0)] = e^{-\beta F(t_0)}$$
(9)

denotes the partition function and $F(t_0)$ the free energy, then $[H(t_0), \rho(t_0)]=0$ and the first measurement of the energy leaves the density matrix unchanged, such that $\bar{\rho}(t_0)=\rho(t_0)$. With Eq. (3) this leads to the characteristic function of work for a canonical initial state that was derived in Ref. [12]. In this case, $G_{t_f,t_0}(u)$ can be continued to an analytical function of *u* for all $0 \le \Im u \le \beta$ [13], where $\Im u$ denotes the imaginary part of *u*. For the particular value $u=i\beta$ the characteristic function yields the mean value of the exponentiated work, $\langle \exp(-\beta w) \rangle$ and the correlation function sat the times t_f and t_0 , resulting in the Jarzynski work theorem

$$\langle e^{-\beta w} \rangle = Z(t_f)/Z(t_0) = \exp\{-\beta [F(t_f) - F(t_0)]\},$$
 (10)

where $Z(t_f) = \text{Tr} \exp[-\beta H(t_f)] = \exp[-\beta F(t_f)]$.

Within the domain of analyticity $S = \{ u | 0 \le \Im u \le \beta \}$ the characteristic functions for the original and the time-reversed protocol are related to each other by the following formula (cf. [13]):

STATISTICS OF WORK PERFORMED ON A FORCED ...

$$G_{t_f,t_0}(u) = \frac{Z(t_f)}{Z(t_0)} G_{t_0,t_f}(-u+i\beta),$$
(11)

where $G_{t_0,t_f}(u)$ refers to processes under the time-reversed protocol $\{H(t)\}_{t_o,t_f}$ starting from the canonical state $Z^{-1}(t_f)\exp[-\beta H(t_f)]$. An inverse Fourier transform leads to the Tasaki-Crooks fluctuation theorem, which relates the probability densities of work $p_{t_o,t_0}(w)$ for a given protocol to the density of the work $p_{t_0,t_f}(w)$ for the time-reversed protocol. This theorem explicitly reads [13]

$$\frac{p_{t_f,t_0}(w)}{p_{t_0,t_f}(-w)} = \frac{Z(t_f)}{Z(t_0)} e^{\beta w} = e^{-\beta [F(t_f) - F(t_0) - w]}.$$
 (12)

B. Fluctuation theorems for microcanonical initial states

A system in a microcanonical state is described by the density matrix

$$\rho(t_0) = \varpi_F^{-1}(t_0) \,\delta(H(t_0) - E), \tag{13}$$

where

$$\boldsymbol{\varpi}_{E}(t_{0}) = \operatorname{Tr} \,\delta(H(t_{0}) - E) = \exp[S(E, t_{0})/k_{B}] \qquad (14)$$

denotes the density of states as a function of the energy E of the system. The density of states can be expressed in terms of the entropy of the system $S_E(t_0)$ provided the spectrum of the system Hamiltonian is sufficiently dense such that the density of states becomes a smooth function on a coarsened energy scale. The microcanonical density matrix commutes with the Hamiltonian $H(t_0)$. Consequently, $\bar{\rho}(t_0)$ and $\rho(t_0)$ coincide.

The microcanonical quantum Crooks theorem assumes the form [14]

$$\frac{p_{t_f,t_0}(E,w)}{p_{t_0,t_f}(E+w,-w)} = \frac{\varpi_{E+w}(t_f)}{\varpi_E(t_0)} = \exp\left(\frac{S(E+w,t_f) - S(E,t_0)}{k_B}\right).$$
(15)

Analogous to the canonical case, it relates the probability density $p_{t_0,t_0}(E,w)$ of work w, for a system starting in a microcanonical state with energy E, to the respective quantity for the time-reversed process starting at energy E+w. This quantum theorem is formally identical to the corresponding classical theorem [19].

From the microcanonical Crooks theorem the probability density of the time-reversed process can be eliminated to yield the so-called entropy-from-work theorem [14], reading

$$\varpi_{E_f}(t_f) = \int dw \ \varpi_{E_f^{-w}}(t_0) p_{t_f,t_0}(E_f - w, w).$$
(16)

This theorem allows one to determine the unknown density of states of a system with Hamiltonian $H(t_f)$ from the known density of states of a reference system $H(t_0)$ by means of the statistics of the work that is performed on the system in a process that leads from the reference system to the final system with unknown density of states. In the case of systems with a sufficiently smooth density of states the corresponding entropy can be determined. For further details see Ref. [14].

IV. DRIVEN HARMONIC OSCILLATOR

To illustrate these concepts we consider an example that allows the analytical construction of the probability of work. Specifically, we consider a harmonic oscillator on which a time-dependent force acts during a finite interval of time. Its time evolution is governed by the Hamiltonian

$$H(t) = \hbar \,\omega a^{\dagger} a + f^{*}(t)a + f(t)a^{\dagger}, \qquad (17)$$

where ω denotes the angular frequency, and a^{\dagger} and a creation and annihilation operators, respectively, which obey the usual commutation relation, i.e., $[a, a^{\dagger}]=1$. The complex driving force f(t) allows for a coupling to position and/or momentum of the oscillator. We assume that f(t) vanishes for times $t \le t_0=0$. It is our aim to study the influence of the initial state $\rho(t_0)$ on the statistics of work performed on the oscillator. The measurement of $H(t_0)=\hbar\omega a^{\dagger}a$ at time $t_0=0$ then yields the result $\hbar\omega n$ with probability

$$p_n = \langle n | \rho(t_0) | n \rangle. \tag{18}$$

Accordingly, the oscillator is found in the state

$$\overline{\rho}(t_0) = \sum_n p_n |n\rangle \langle n| \tag{19}$$

immediately after this measurement. Substituting this density matrix in the general expression for the characteristic function, Eq. (3), one obtains

$$G_{t_{f},t_{0}}(u) = \sum_{n} p_{n} e^{-iu\hbar\omega n} \langle n | e^{iuH_{H}(t_{f})} | n \rangle.$$
(20)

For the driven harmonic oscillator the diagonal matrix element of the exponentiated Hamiltonian $H_H(t_f)$ can be determined [17]. For details see Appendix B. With the expression (B14) for the matrix element $\langle n|\exp[iH_H(t_f)]|n\rangle$ we find

$$G_{t_{f},t_{0}}(u) = e^{iu|f(t_{f})|^{2/(\hbar\omega)}} \exp[(e^{iu\hbar\omega} - 1)|z|^{2}]$$

$$\times \sum_{n=0}^{\infty} \sum_{k=0}^{n} p_{n} {n \choose k} \frac{|z|^{2(n-k)}}{(n-k)!} e^{-iu\hbar\omega(n-k)} (e^{iu\hbar\omega} - 1)^{2(n-k)}$$

$$= e^{iu|f(t_{f})|^{2/(\hbar\omega)}} \exp[(e^{iu\hbar\omega} - 1)|z|^{2}]$$

$$\times \sum_{n=0}^{\infty} p_{n} L_{n} \left(4|z|^{2} \sin^{2}\frac{\hbar\omega u}{2}\right), \qquad (21)$$

where $|f(t_f)|^2/(\hbar\omega)$ denotes a uniform shift of the spectrum of the harmonic oscillator due to the presence of the external force [cf. Eq. (B9)] and

$$z = \frac{1}{\hbar\omega} \int_0^{t_f} ds \, \dot{f}(s) \exp(i\omega s) \tag{22}$$

is a dimensionless functional of the driving force f(t) [cf. Eq. (B7)]. This dimensionless quantity vanishes in particular for all-quasistatic forcings, i.e., if the force changes only very slowly with $f(t)=g(t/t_f)$ for $t_f \rightarrow \infty$, where $g(\tau)$ is a continuously differentiable function of $\tau \in [0, 1]$. We hence call z(t)

the *rapidity parameter* of the force protocol. Finally, $L_n(x) = \sum_{k=0}^{n} {n \choose k} (-x)^k / k!$ denotes the Laguerre polynomial of order n [21].

Introducing the cumulant generating function $K(u) = \ln G(u)$, one obtains the cumulants of work k_n as the *n*th derivatives of K(u) with respect to *u* taken at u=0 [22], i.e., $k_n=(-i)^n d^n K(0)/du^n$. The first four cumulants become

$$k_1 = \langle w \rangle = \frac{|f(t_f)|^2}{\hbar \omega} + \hbar \omega |z|^2, \qquad (23)$$

$$k_2 = \langle w^2 \rangle - \langle w \rangle^2 = 2(\hbar \omega)^2 |z|^2 \left(\langle a^{\dagger} a \rangle_0 + \frac{1}{2} \right), \qquad (24)$$

$$k_3 = \langle w^3 \rangle - 3 \langle w^2 \rangle \langle w \rangle + 2 \langle w \rangle^3 = (\hbar \omega)^3 |z|^2, \qquad (25)$$

$$k_{4} = \langle w^{4} \rangle - 4 \langle w^{3} \rangle \langle w \rangle - 3 \langle w^{2} \rangle^{2} + 12 \langle w^{2} \rangle \langle w \rangle^{2} - 6 \langle w \rangle^{4}$$

$$= (\hbar \omega)^{4} |z|^{2} \{1 + 4 \langle a^{\dagger} a \rangle_{0} + 6[\langle a^{\dagger} a (a^{\dagger} a - 1) \rangle_{0} - 2 \langle a^{\dagger} a \rangle_{0}] |z|^{2} \}.$$

(26)

The odd cumulants of the work are independent of the initial preparation. The even cumulants depend on the factorial moments of the number operator $a^{\dagger}a$ with respect to the initial state $\bar{\rho}(t_0)$ such as $\langle a^{\dagger}a \rangle_0 = \sum_n np_n$ and $\langle a^{\dagger}a(a^{\dagger}a-1) \rangle_0 = \sum_n n(n-1)p_n$, where p_n is defined in Eq. (18). Moreover, all cumulants apart from the first one vanish for forcings with z=0. This holds true in particular for all quasistatic force characteristics. The underlying work probability density then shrinks to a δ function at $w = |f(t_f)|^2 / (\hbar \omega)$.

In general, the work probability density follows from the characteristic function by means of an inverse Fourier transformation. Rather than the characteristic function itself, we first consider the function $\mathcal{G}(u) \equiv \exp[-iu|f(t_f)|^2/(\hbar\omega)] \times G_{t_f,t_0}(u)$. Upon expanding $\exp[|z|^2\exp(iu\hbar\omega)]$ into a series of powers of $|z|^2$, we obtain for $\mathcal{G}(u)$ a Laurent series in the variable $\exp[iu\hbar\omega]$. The inverse Fourier transformation is given by a series of δ functions $\delta(w-\hbar\omega r)$, with $r \in \mathbb{Z}$, with weights

$$q_{r} = e^{-|z|^{2}} \sum_{m,n=0}^{\infty} \sum_{k=0}^{n} \sum_{l=0}^{2k} (-1)^{2k-l} p_{n} \frac{|z|^{2(k+m)}}{m!k!} \binom{n}{k} \binom{2k}{l} \delta_{l+m,k+r}$$

$$= e^{-|z|^{2}} \sum_{n=0}^{\infty} \sum_{k=0}^{n} \sum_{l=0}^{\min(k+r,2k)} (-1)^{2k-l} p_{n} \frac{|z|^{2(2k+r-l)}}{(k+r-l)!k!} \binom{n}{k} \binom{2k}{l}.$$
(27)

The factor $\exp[-iu|f(t_f)|^2/(\hbar\omega)]$, by which $\mathcal{G}(u)$ has to be multiplied to yield $G_{t_f,t_0}(u)$, gives rise to a constant shift such that the probability density of work performed on a harmonic oscillator becomes

$$p_{t_{f}t_{0}}(w) = \sum_{r} q_{r} \delta \left(w - \left(\hbar \omega r + \frac{|f(t_{f})|^{2}}{\hbar \omega} \right) \right).$$
(28)

In the next section we will investigate the influence of the initial state on the statistics of the work.

A. Distributions of work for different initial states

As particular examples of initial states we will discuss microcanonical, canonical, and coherent states.

1. Microcanonical initial state

For a microcanonical initial state with energy $\hbar \omega n_0$ the density matrix becomes

$$\rho(t_0) = \overline{\rho}(t_0) = |n_0\rangle \langle n_0|. \tag{29}$$

The characteristic function then reads

$$G_{t_f,t_0}^{\rm mc}(n_0,u) = e^{iu[f(t_f)]^2/(\hbar\omega)} \exp[(e^{iu\hbar\omega} - 1)|z|^2] \times L_{n_0}\left(4|z|^2\sin^2\frac{\hbar\omega u}{2}\right)$$
(30)

and, accordingly, the probability $q_r^{\rm mc}(n_0)$ to find a change of energy by $w = \hbar \omega r + |f(t_f)|^2 / (\hbar \omega)$ emerges as

$$q_r^{\rm mc}(n_0) = e^{-|z|^2} \sum_{k=0}^{n_0} \sum_{l=0}^{\min(k+r,2k)} \frac{(-1)^{2k-l}}{(k+r-l)!k!} \binom{n}{k} \binom{2k}{l} |z|^{2(2k+r-l)}.$$
(31)

As expected from the behavior of the moments, all probabilities $q_r^{\text{mc}}(n_0)$ with $r \neq 0$ vanish for quasistatic forcing, i.e., if $z \rightarrow 0$. The dependence of $q_r^{\text{mc}}(n_0)$ on the parameter z is displayed in Fig. 1 for $n_0=0$ and 3 as well as for the eight lowest values of r. With increasing values of the rapidity parameter z the distribution is becoming broader.

For the fixed value of |z|=2 the distribution $q_r^{\rm mc}(n_0)$ is compared for the three initial states with $n_0=0$, 10, and 30 in Fig. 2. With increasing value of n_0 the distributions become broader. They develop a slightly asymmetric shape with higher peaks at negative values of r compared to those at positive r values. Between these dominant peaks the probability still displays pronounced variations.

For a harmonic oscillator, the microcanonical Crooks theorem reduces to the relation $q_r^{\rm mc}(n) = q_{-r}^{\rm mc}(n+r)$. One can prove that this symmetry is satisfied by the probabilities $q_r^{\rm mc}(n)$ given by Eq. (31). As a consequence, the ratio $q_r^{\rm mc}(n)/q_{-r}^{\rm mc}(n+r)$ is unity independently of the actual values of the initial energy, the work, and the force protocol as given by *n*, *r*, and *z*, respectively.

2. Canonical initial state

For a canonical density matrix

$$\rho(t_0) = (1 - e^{-\beta\hbar\omega})e^{-\beta\hbar\omega a^{\dagger}a}$$
(32)

the initial states are distributed according to $p_n = e^{-\beta\hbar\omega n}(1 - e^{-\beta\hbar\omega})$. This allows one to write the sum over *n* in the characteristic function (21) in terms of the generating function of the Laguerre polynomials (cf. [21]) yielding the expression

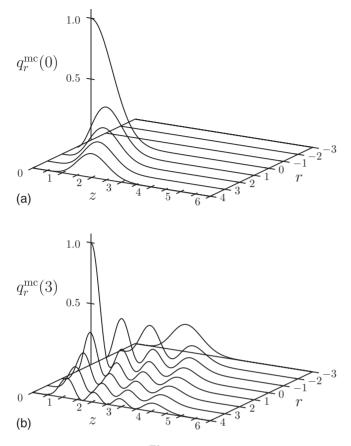


FIG. 1. Probabilities $q_r^{mc}(n_0)$ for two microcanonical initial states with $n_0=0$ (a) and 3 (b) are depicted for $r=-3, \ldots, 4$, as functions of the rapidity parameter z defined in Eq. (B7). In both cases the distribution collapses at r=0 for qausi—static forcing, corresponding to |z|=0, and broadens with increasing |z|. Obviously, when starting in the ground state the oscillator cannot deliver work, whence the probability for negative r strictly vanishes. "Stimulated emission" becomes possible from an excited state at finite driving rapidity z, leading to nonzero probabilities $q_r^{mc}(n_0)$ at negative values of r in (b).

$$G_{t_f t_0}^{c}(\beta, u) = \exp\left(\frac{iu|f(t_f)|^2}{\hbar\omega} + (e^{iu\hbar\omega} - 1)|z|^2 - 4|z|^2 \frac{\sin^2(\hbar\omega u/2)}{e^{\beta\hbar\omega} - 1}\right).$$
(33)

Putting $u=i\beta$, one finds that the two terms in the exponent that are proportional to $|z|^2$ cancel each other, such that one obtains

$$\langle e^{-\beta w} \rangle = G^{c}_{t_{f},t_{0}}(\beta, i\beta) = \exp[-\beta |f(t_{f})|^{2}/(\hbar\omega)].$$
(34)

The free energy difference of two oscillators with Hamiltonians $H(t_0) = \hbar \omega a^{\dagger} a$ and $H(t_f) = \hbar \omega a^{\dagger} a + f^*(t_f) a + f(t) a^{\dagger}$, each one staying in a canonical state at the temperature β , is given by $\Delta F = F(t_f) - F(t_0) = |f(t_f)|^2 / (\hbar \omega)$. Hence, Eq. (34) agrees with Jarzynski's work theorem.

The probability $q_r^c(\hat{\beta})$ to find the work $w = \hbar \omega r + |f(t_f)|^2 / (\hbar \omega)$ if the system starts in a canonical state becomes

$$q_{r}^{c}(\tilde{\beta}) = e^{-|z|^{2}}(1 - e^{-\tilde{\beta}})\sum_{n=0}^{\infty}\sum_{k=0}^{n}\sum_{l=0}^{\min(k+r,2k)}(-1)^{l}e^{-\tilde{\beta}n} \times \frac{|z|^{2(2k+r-l)}}{(k+r-l)!k!}\binom{n}{k}\binom{2k}{l},$$
(35)

where $\tilde{\beta} = \beta \hbar \omega$ denotes the inverse dimensionless temperature of the initial state. The expression for $q_r^c(\tilde{\beta})$ can be further simplified to read

$$q_r^{\rm c}(\tilde{\beta}) = e^{-|z|^2 \coth(\tilde{\beta}/2)} e^{\tilde{\beta}r/2} I_r \left(\frac{|z|^2}{\sinh \tilde{\beta}/2}\right),\tag{36}$$

where $I_{\nu}(x)$ denotes the modified Bessel function of the first kind of order ν [21]. For details of the derivation see Appendix C.

Note that the following detailed-balance-like symmetry relation exists:

$$q_{-r}^{\rm c}(\tilde{\beta}) = e^{-\beta r} q_r^{\rm c}(\tilde{\beta}), \qquad (37)$$

relating the occurrence of positive and negative work. Figure 3 illustrates this relation, which is closely connected to the Tasaki-Crooks theorem (12), as demonstrated at the end of this section. In Fig. 4 the *z* dependence of $q_r^c(\tilde{\beta})$ for $\tilde{\beta} = \ln(4/3)$ is compared for a few small values of *r*. One finds that, because of the average over the canonical initial distribution, the multipeaked structure of the microcanonical distribution as a function of the rapidity parameter |z| disappears, and only a single peak remains for each value of *r*. The temperature dependence of the work distribution is illustrated in Fig. 5.

Finally, we verify the validity of the Tasaki-Crooks theorem (12) for a driven oscillator. For this purpose we consider the probability density $p_{t_0,t_f}(-w)$ for the time-reversed protocol. Since the absolute values of the rapidity parameters coincide for the original and the time-reversed protocols, the probability density of work for the reversed protocols becomes

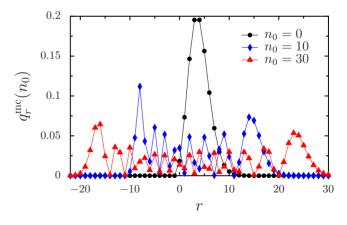


FIG. 2. (Color online) Probabilities $q_r^{\rm mc}(n_0)$ for a microcanonical initial state with $n_0=0$ (circles), 10 (diamonds), and 30 (triangles) are compared for a fixed rapidity parameter |z|=2 and $r=-22,\ldots,30$. The lines serve as a guide for the eye.

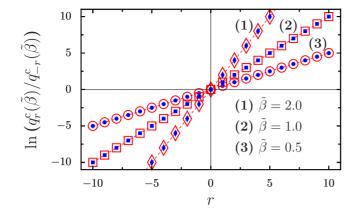


FIG. 3. (Color online) Natural logarithm of the probability ratio of positive and negative transferred work resulting from Eq. (36) as a function of r for different dimensionless temperatures $\tilde{\beta} = \beta/\hbar\omega$ =0.5,1,2 (circles, squares, lozenges) and different rapidity parameters z=1,2 (large open, small filled symbols). The symmetry relation (37) implies a linear law with inclination $\tilde{\beta}$ (thin straight broken lines) which is independent of the rapidity parameter. The agreement is perfect.

$$p_{t_0,t_f}(-w) = \sum_{r=-\infty}^{\infty} q_r^c(\beta) \delta\left(-w - \left(\hbar\omega r - \frac{|f(t_f)|^2}{\hbar\omega}\right)\right), \quad (38)$$

where we took into account the overall shift of the spectrum by the reversed protocol as $-|f(t_f)|/(\hbar\omega)$. Multiplying both sides of Eq. (38) with $\exp[-\beta(\Delta F - w)] = \exp\{-\beta[|f(t_f)|^2/(\hbar\omega) - w]\}$ and using the symmetry (37), one obtains

$$\begin{split} e^{-\beta(\Delta F - w)} p_{t_0, t_f}(-w) &= \sum_r e^{-\beta[|f(t_f)|^2/(\hbar\omega) - w]} q_r^c(\widetilde{\beta}) \\ &\times \delta \left(-w - \left(\hbar \omega r - \frac{|f(t_f)|^2}{\hbar \omega} \right) \right) \\ &= \sum_r e^{\widetilde{\beta} r} q_r^c(\widetilde{\beta}) \delta \left(w + \left(\hbar \omega r - \frac{|f(t_f)|^2}{\hbar \omega} \right) \right) \end{split}$$

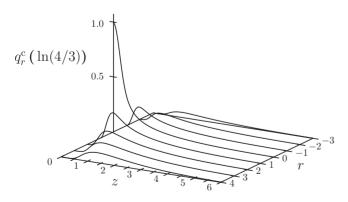


FIG. 4. Probabilities $q_r^c[\tilde{\beta}=\ln(4/3)]$ for a canonical initial state for $r=-3, \ldots, 4$ as functions of the parameter z. For the sake of comparability, the dimensionless inverse temperature is chosen such that the average energy in the initial state coincides with the energy $3\hbar\omega$ of the microcanonical state in Fig. 1(b).

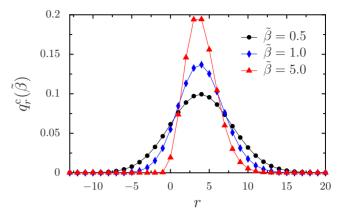


FIG. 5. (Color online) Probabilities $q_r^c(\tilde{\beta})$ for a canonical initial state as functions of *r* for |z|=2 and different values of the dimensionless inverse temperature $\tilde{\beta}=0.5$ (circles), 1 (diamonds), and 5 (triangles). The lines serve as a guide for the eye.

$$=p_{t_{k}t_{0}}(w), \tag{39}$$

in accordance with the Tasaki-Crooks theorem (12). Conversely, if the Tasaki-Crooks theorem holds for a discrete work distribution of the form (28), then the detailed-balance-like relation (37) follows for the probabilities $q_r^c(\tilde{\beta})$.

3. Coherent initial state

An oscillator prepared in a coherent state $|\alpha\rangle$ is described by the density matrix

$$\rho(t_0) = |\alpha\rangle \langle \alpha|, \tag{40}$$

where

$$|\alpha\rangle = e^{\alpha a^{\top} + \alpha^* a} |0\rangle, \tag{41}$$

and $|0\rangle$ is the normalized ground state of the oscillator satisfying $a|0\rangle=0$. Note that the coherent state density matrix does *not* commute with the Hamiltonian $H(t_0)$. The measurement of $H(t_0)$ modifies the coherent state (40) by projecting it onto the eigenstates $|n\rangle=(a^{\dagger})^n/\sqrt{n!}|0\rangle$ of this Hamiltonian, leading to

$$\overline{p}(t_0) = e^{-|\alpha|^2} \sum_n \frac{|\alpha|^{2n}}{n!} |n\rangle \langle n|.$$
(42)

This implies a Poissonian distribution of the respective energy eigenvalues $\hbar \omega n$,

$$p_n^{\rm cs} = \frac{|\alpha|^{2n}}{n!} e^{-|\alpha|^2},\tag{43}$$

which yields for the characteristic function of work (21) a closed expression of the form

$$G_{t_{f},t_{0}}^{cs}(\alpha,u) = \exp\left(\frac{iu|f(t_{f})|^{2}}{\hbar\omega} + |z|^{2}(e^{i\hbar\omega u} - 1)\right)$$
$$\times J_{0}\left(4\left|\alpha z \sin\frac{\hbar\omega u}{2}\right|\right), \tag{44}$$

where $J_0(x)$ is the Bessel function of order zero (cf. Ref

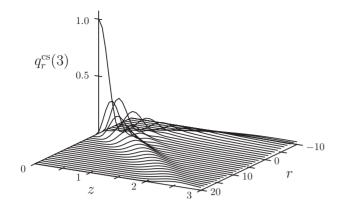


FIG. 6. Probabilities $q_r^{cs}(\alpha)$ for a coherent state with parameter $|\alpha|=3$ for $r=-10,\ldots,20$ as functions of *z*.

[21]). For the probability $q_r^{cs}(\alpha)$ of work one obtains with Eq. (27)

$$q_r^{\rm cs}(\alpha) = e^{-|z|^2} \sum_{m=0}^{\infty} \frac{|z|^{2m} |\alpha z|^{2|m-r|}}{m! (|m-r|!)^2} {}_1F_2\left(|m-r| + \frac{1}{2}; |m-r| + 1, 2|m-r| + 1; -4|\alpha z|^2\right),$$
(45)

where ${}_{1}F_{2}(a;b,x;x)$ denotes a generalized hypergeometric function [21]. For details of the derivation, see Appendix D.

The dependence of the probabilities $q_r^{cs}(\alpha)$ on the rapidity parameter |z| is illustrated in Fig. 6 for *r* values ranging from -10 to 20. Increasing values of z lead to a broadening of the distribution and also to a shift toward larger values of r; see also Fig. 7(b). This broadening and shift is in accordance with Eq. (23) and (24) for the first two cumulants of the work, which both increase with $|z|^2$. Figure 7(a) shows the dependence of the probabilities $q_r^{cs}(\alpha)$ on the parameter α . Increasing α also leads to a broadening of the work distribution without influencing its mean value [cf. also Eq. (23)]. In Fig. 8 the probabilities q_r are depicted for different initial states. In one case the oscillator is initially prepared in a canonical state at inverse dimensionless temperature β $=\beta\hbar\omega=0.1$. In the other case, the oscillator stays in a coherent state $|\alpha\rangle$, where the absolute value of α is chosen such that the mean excitation number is the same for both states, i.e., $|\alpha|^2 = \exp(-\beta\hbar\omega)/[1 - \exp(-\beta\hbar\omega)]$. For $\beta\hbar\omega = 0.1$ one finds $|\alpha|^2 \approx 9.51$. The two oscillators then are subjected to protocols with the same rapidity parameter |z|=2. According to Eqs. (23) and (24) the first two moments of the work performed on the oscillators coincide. Yet the distribution of weight factors $q_r^{\rm c}(\tilde{\beta})$ and $q_r^{\rm cs}(\alpha)$ distinctly differ. Whereas the distribution is pronouncedly bimodal in the case of the coherent state, it is unimodal for the canonical state. The weight factors $q_r^{c}(\hat{\beta})$ almost perfectly fall onto a Gaussian probability density which has the same first two moments as the discrete distribution given by q_r .

V. CONCLUSIONS

In this work we studied the statistics of work performed on an externally driven quantum mechanical oscillator by

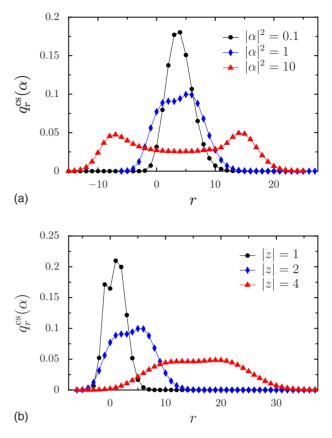


FIG. 7. (Color online) Distribution of work performed on an oscillator which initially is prepared in a coherent state $|\alpha\rangle$ for different values of α in (a) and of the rapidity parameter z in (b). In (a) the rapidity parameter has the value |z|=2. In (b) the coherent state parameter has the value $|\alpha|^2=1$.

means of a correlation function expression for the characteristic function of the work. We demonstrated that this particular expression indeed always represents a proper characteristic function of a random variable, which is the performed

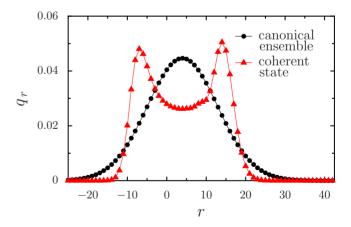


FIG. 8. (Color online) Distribution of work compared for a canonical and a coherent initial state subject to the same force protocol with rapidity parameter z=2. With $\beta\hbar\omega=0.1$ and $|\alpha|^2\approx9.51$, the expectation values of the energies agree in the two initial states such that according to Eqs. (23) and (24) the first and second moments of the work also coincide. Still the distributions of work greatly differ from each other.

work in the present context. The proof given here is based on Bochner's theorem. Note that it holds for general quantum mechanical systems, not only for harmonic oscillators.

The considered force linearly couples to the position and momentum of the oscillator. It may describe the influence of an electric field on charged particles in a parabolic trap or the external forcing of a single electromagnetic cavity mode. For this type of additive forcing, the frequency of the oscillator remains unchanged and therefore the level spacing of the eigenvalues of the Hamiltonian is not influenced by the force. The spectrum is only shifted as a whole. As a consequence the work performed on the oscillator is, as a positive or negative integer multiple of the level spacing, a discrete random variable. We determined the first few cumulants of the work for arbitrary force protocols and initial states. A complementary study for a parametrically forced oscillator was recently performed by Deffner and Lutz [15].

It turns out that for the harmonic oscillator the statistics of work depends on the force protocol $\{f(t)\}_{t_f,t_0}$ only through two real parameters, which are (i) the shift of the spectrum, given by $L(t_f) = |f(t_f)|^2 / (\hbar \omega)$, and (ii) the absolute value of the dimensionless quantity $z = \int_{t_0}^{t_f} f(s) \exp(i\omega s)$. This parameter vanishes for all quasistatic processes and therefore presents a measure of the rapidity of the force protocol. While the presence of $L(t_f)$ only causes an overall shift of the possible values of the work, the rapidity parameter |z| also influences its distribution. Typically, the distributions move toward larger values of work w and become broader with increasing rapidity |z|, indicating a more violent impact on the oscillator.

We also demonstrated that different initial states of the system such as microcanonical, canonical, or coherent states have a large influence on the work statistics. We further note that two different initial density matrices with the same diagonal elements with respect to the energy eigenbasis of the Hamiltonian $H(t_0)$ lead to identical work distributions even though the two density matrices may be very different in other respects. For example, the coherent pure state $|\alpha\rangle\langle\alpha|$ and the mixed state $\exp(-|\alpha|^{2n})\Sigma_n|\alpha|^2/n!|n\rangle\langle n|$ cannot be distinguished by means of their respective work statistics. This statistics is also insensitive to the phase of a coherent state.

ACKNOWLEDGMENTS

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APPENDIX A: PROOF OF THE PROPERTIES OF $G_{t_0 t_0}(u, v)$

We prove that the conditions of Bochner's theorem are satisfied, and consequently $G_{t_{f},t_0}(u)$ is a proper characteristic function.

Proof of property (i): $G_{t_f,t_0}(u)$ is a continuous function of u. The Hamiltonian operators at the two times of measurement t_0 and t_f are self-adjoint operators. According to the

theorem of Stone [20], each of the exponential operators $\exp[-iuH(t_0)]$ and $\exp[iuH_H(t_f)]$ forms a strongly continuous one-parameter group of unitary operators with parameter *u*. As the trace of a product of two strongly continuous operator valued functions of *u* with the density operator $\overline{\rho}(t_0)$, which is a trace class operator and independent of *u*, the characteristic function (3) is a continuous function of *u*.

Proof of property (ii): $G_{t_f,t_0}(u)$ is a positive definite function of *u*. Using the cyclic invariance of the trace and the fact that $H(t_0)$ and $\bar{\rho}(t_0)$ commute with each other, we can rewrite the left-hand side of the inequality (7) as

$$\sum_{i,j}^{n} G_{t_{f},t_{0}}(u_{i}-u_{j})z_{i}^{*}z_{j} = \sum_{i,j}^{n} \operatorname{Tr} e^{i(u_{i}-u_{j})H_{H}(t_{f})}e^{-i(u_{i}-u_{j})H(t_{0})}\overline{\rho}(t_{0})z_{i}^{*}z_{j}$$
$$= \operatorname{Tr} A^{\dagger}A\overline{\rho}(t_{0}) \ge 0, \qquad (A1)$$

where

$$A = \sum_{i} z_{i}^{n} e^{-iu_{i}H_{H}(t_{f})} e^{iu_{i}H(t_{0})}$$
(A2)

is a bounded operator and A^{\dagger} its adjoint. The last inequality in (A1) immediately follows from the positivity of $A^{\dagger}A$ and of the density matrix $\bar{\rho}(t_0)$.

Proof of property (iii): $G_{t_f,t_0}(0)=1$. For u=0 the exponential operators $\exp[-iuH(t_0)]$ and $\exp[iuH_H(t_f)]$ become unity. By means of Eqs. (5) and (6) the trace over the density matrix $\overline{\rho}(t_0)$ reduces to the trace of the initial density matrix $\rho(t_0)$, which is 1.

APPENDIX B: THE MATRIX ELEMENT $\langle n | \exp[i u H_H(t_f)] | n \rangle$

The total time rate of change of the Hamiltonian $H_H(t)$ coincides with its partial derivative with respect to time. Hence, we obtain with Eq. (17) for the driven oscillator

$$\frac{dH_H(t)}{dt} = \dot{f}^*(t)a_H(t) - \dot{f}(t)a_H^{\dagger}(t),$$
(B1)

where $a_H(t)$ and $a_H^{\dagger}(t)$ denote annihilation and creation operators, respectively, in the Heisenberg picture, which are given by

$$a_{H}(t) = e^{-i\omega t}a - \frac{i}{\hbar} \int_{0}^{t} ds \ e^{-i\omega(t-s)} f(s)$$
(B2)

and

$$a_{H}^{\dagger}(t) = e^{i\omega t}a^{\dagger} + \frac{i}{\hbar} \int_{0}^{t} ds \ e^{i\omega(t-s)} f^{*}(s). \tag{B3}$$

This yields for $H_H(t_f)$

$$H_{H}(t_{f}) = \hbar \omega a^{\dagger} a + B^{*}(t_{f})a + B(t_{f})a^{\dagger} + C(t),$$
 (B4)

where

$$B(t_f) = \int_0^{t_f} ds \, \dot{f}(s) e^{i\omega s}$$

$$C(t_{f}) = \frac{i}{\hbar} \int_{0}^{t_{f}} ds \int_{0}^{s} ds' [\dot{f}(s)f^{*}(s')e^{i\omega(s-s')} - \dot{f}^{*}(s)f(s')e^{-i\omega(s-s')}].$$
 (B5)

The unitary operator

$$V = e^{za^{\dagger} - z^*a} \tag{B6}$$

with

$$z = \frac{B(t_f)}{\hbar\omega} \tag{B7}$$

transforms $H_H(t)$ into

$$VH_H(t_f)V^{\dagger} = \hbar \omega a^{\dagger} a + L(t_f), \qquad (B8)$$

where

$$L(t_f) = C(t_f) - \frac{|B(t_f)|^2}{\hbar\omega} = \frac{|f(t_f)|^2}{\hbar\omega}.$$
 (B9)

Note that V induces a shift of the creation and annihilation operators,

$$VaV^{\dagger} = a - z, \quad Va^{\dagger}V^{\dagger} = a^{\dagger} - z^*, \tag{B10}$$

and further note that, when acting on the ground state $|0\rangle$ with $a|0\rangle=0$, the operator V yields the coherent state $|z\rangle$, i.e.,

$$V|0\rangle = |z\rangle. \tag{B11}$$

One finds with these properties

$$\langle n|e^{iuH_{H}(t_{f})}|n\rangle = \frac{1}{n!} \langle z|(a-z)^{n} e^{iu\hbar\omega a^{\dagger}a + iuL(t_{f})} (a^{\dagger}-z^{*})^{n}|z\rangle$$
$$= \frac{1}{n!} e^{iuL(t_{f})} \frac{\partial^{2n}}{\partial x^{n} \partial y^{n}}$$
$$\times \langle z|e^{x(a-z)} e^{iu\hbar\omega a^{+}a} e^{y(a^{+}-z^{*})}|z\rangle|_{x=v=0}.$$
(B12)

Here we have introduced the auxiliary variables x and y

which allow us to represent the *n*th powers of shifted creation and annihilation operators by derivatives of the corresponding order. The scalar function $e^{-i(xz+yz^*)}$ can be taken out of the scalar product and the remaining operator can be brought into normal order. It then becomes [23]

$$e^{xa}e^{iu\hbar\omega a^{\dagger}a}e^{ya^{\dagger}} = \mathcal{N}\{\exp[(e^{iu\hbar\omega} - 1)a^{\dagger}a + e^{iu\hbar\omega}(xa + ya^{\dagger} + xy)]\}, \quad (B13)$$

where under the normal ordering operator \mathcal{N} all creation operators stand left of the annihilation operators. The matrix element with respect to the coherent state $|z\rangle$ can be read off, yielding

$$\langle n | e^{iuH_{H}(t_{f})} | n \rangle = \frac{1}{n!} e^{iuL(t_{f})} \exp[(e^{iu\hbar\omega} - 1)|z|^{2}] \frac{\partial^{2n}}{\partial x^{n} \partial y^{n}}$$

$$\times \exp[(e^{iu\hbar\omega} - 1)(xz + yz^{*}) + e^{iu\hbar\omega}xy]|_{x=y=0}$$

$$= \frac{1}{n!} e^{iuL(t_{f})} \exp[(e^{iu\hbar\omega} - 1)|z|^{2}] \frac{\partial^{n}}{\partial y^{n}}$$

$$\times [(e^{iu\hbar\omega} - 1)z + e^{iu\eta\omega}y]^{n} \exp[(e^{iu\hbar\omega} - 1)$$

$$\times (|z|^{2} + yz^{*})]|_{y=0}$$

$$= e^{iu[f(t_{f})]^{2/(\hbar\omega)}} \exp[(e^{iu\hbar\omega} - 1)|z|^{2}]$$

$$\times \sum_{k=0}^{n} {n \choose k} \frac{|z|^{2(n-k)}}{(n-k)!} e^{iu\hbar\omega k} (e^{iu\hbar\omega} - 1)^{2(n-k)}.$$

$$(B14)$$

APPENDIX C: WORK DISTRIBUTION FOR A CANONICAL INITIAL STATE

To determine the expression (36) for the work distribution $q^{c}(\tilde{\beta})$, we start from the general expression given in the first equality of Eq. (27). Interchanging the summation over the indices *n* and *k*, we obtain

$$q_r^c(\tilde{\beta}) = e^{-|z|^2} \sum_{m,k=0}^{\infty} \sum_{l=0}^{2k} (-1)^l \frac{|z|^{2(k+m)}}{m!k!} \binom{2k}{l} \delta_{l+m,k+r} \sum_{n=k}^{\infty} \frac{e^{-\beta n}}{1 - e^{-\tilde{\beta}}} \binom{n}{k}$$

...

$$\stackrel{(1)}{=} e^{-|z|^2} \sum_{m,k=0}^{\infty} \sum_{l=0}^{2k} (-1)^l \frac{|z|^{2(k+m)}}{m!k!} \binom{2k}{l} \left(\frac{1}{e^{\tilde{\beta}} - 1}\right)^k \delta_{l+m,k+r}$$

$$\stackrel{(2)}{=} (-1)^{r} e^{-|z|^{2}} \sum_{m=0}^{\infty} \frac{(-|z|^{2})^{m}}{m!} \sum_{k=|m-r|}^{\infty} \frac{[-|z|^{2}/(e^{\tilde{\beta}}-1)]^{k}}{k!} \binom{2k}{k+r-m}$$

In the first step $(=)^{(1)}$ we performed the sum on *n* according to

$$\sum_{n=k}^{\infty} \frac{x^k}{1-x} {n \choose k} = \left(\frac{x}{1-x}\right)^k \tag{C2}$$

(2)

(cf. Ref. [24], formula 5.2.11.3). In the second step (=) the Kronecker δ is used to perform the sum over *k*. The third $\binom{(3)}{2}$

step (=) is based on the relation

$$\sum_{k=|l|}^{\infty} \frac{x^{k}}{k!} \binom{2k}{k+l} = e^{2x} I_{|l|}(2x)$$
(C3)

valid for integer *l*. Here $I_{\nu}(x)$ denotes the modified Bessel function of the first kind of order ν . With $I_{\nu}(-x) = (-1)^{\nu}I_{\nu}(x)$, where ν is an integer, we come to the right-hand

side of the equality (=). In the next step the sum on *m* is rewritten. The term in the square brackets vanishes because $I_{\nu}(x)$ is an even function of order ν . The remaining sum can be performed by means of the identity

$$\sum_{k=0}^{\infty} \frac{t^k}{k!} I_{\nu-k}(x) = \left(\frac{2t}{x} + 1\right)^{\nu/2} I_{\nu}(\sqrt{x^2 + 2tx})$$
(C4)

(cf. [24] 5.8.3.1). This leads to the final result given in Eq. (36).

APPENDIX D: WORK DISTRIBUTION FOR A COHERENT INITIAL STATE EQ. (45)

Starting from Eq. (27), we may proceed in an analogous way as in the case of a canonical initial state; cf. Appendix C. According to Eq. (43) a Poissonian average over the binomial $\binom{n}{k}$ has to be performed instead of the geometric average in the first step of Eq. (C1). This yields

$$\sum_{n=k}^{\infty} \frac{|\alpha|^{2n}}{n!} e^{-|\alpha|^2} \binom{n}{k} = \frac{|\alpha|^{2k}}{k!}.$$
 (D1)

Next the Kronnecker δ is used to perform the sum over *l*, leaving one with two sums of which the inner one over *k* can be expressed in terms of a generalized hypergeometric function [21], to become

$$\sum_{k=|m-r|}^{\infty} \frac{(-|\alpha z|^2)^k}{(k!)^2} {2k \choose k+r-m}$$

= $\frac{(-|\alpha z|^2)^{|m-r|}}{(|m-r|!)^2} {}_1F_2 \Big(|m-r| + \frac{1}{2}; |m-r| + 1; -4|\alpha z|^2 \Big).$ (D2)

This immediately leads to the expression in Eq. (45).

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