

Nonequilibrium Green's Function's Approach to the Calculation of Work Statistics

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The calculation of work distributions in a quantum many-body system is of significant importance and also of formidable difficulty in the field of nonequilibrium quantum statistical mechanics. To solve this problem, inspired by the Schwinger-Keldysh formalism, we propose the contour-integral formulation for work statistics. Based on this contour integral, we show how to do the perturbation expansion of the characteristic function of work (CFW) and obtain the approximate expression of the CFW to the second order of the work parameter for an arbitrary system under a perturbative protocol. We also demonstrate the validity of fluctuation theorems by utilizing the Kubo-Martin-Schwinger condition. Finally, we use noninteracting identical particles in a forced harmonic potential as an example to demonstrate the powerfulness of our approach.

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Introduction.—In the past 25 years or so, the development of stochastic thermodynamics and the discovery of fluctuation theorems have revolutionized our understanding about nonequilibrium thermodynamics [1–4]. In these studies, a key quantity is the probability distribution of work in an arbitrary nonequilibrium process, which encodes essential information about the nonequilibrium process analogous to the partition function encoding essential information about an equilibrium state [5–8]. For a closed quantum system, the trajectory work is defined as the difference between the results of the projective measurements over the system's energy before and after the driving protocol [9–11]. Accordingly, the characteristic function of work [CFW; the Fourier transform of the work distribution $P(w)$] reads [11]

$$\chi(v) = \int dw P(w) e^{ivw} = \text{Tr}[\hat{U}^\dagger(t) e^{iv\hat{H}(t)} \hat{U}(t) e^{-iv\hat{H}(0)} \hat{\rho}], \quad (1)$$

where $\hat{\rho}$ denotes the initial state, $\hat{H}(0)$ and $\hat{H}(t)$ denote the Hamiltonians before and after the driving protocol, and $\hat{U}(s)$ denotes the time-evolution operator corresponding to a time-dependent Hamiltonian $\hat{H}(s)$, $s \in [0, t]$. The CFW is a powerful tool to study the nonequilibrium physics of a quantum system, since it appears not only in stochastic thermodynamics, but also in Loschmidt echoes [12,13], Kibble-Zurek mechanism [14], dynamical quantum phase transitions [15,16], and many other fields. Hence, to efficiently calculate the CFW becomes one of the most important problems in this field.

Nevertheless, it is usually a very challenging task to calculate the CFW for an arbitrary nonequilibrium

protocol, especially for quantum many-body systems, due to the complicated nonequilibrium dynamics. In the literature, there are a few results about the CFW, but mostly focusing on special models and are studied case by case [8,17–26]. For example, in Refs. [8,26], the perturbation expansion is applied to the calculation of the work distributions of a quantum scalar field for perturbative protocols. For quantum systems described by quadratic Hamiltonians, Ref. [27] proposed a general method for solving the CFW under an arbitrary driving protocol by utilizing the group-representation theory. Nevertheless, for a general model beyond the quadratic Hamiltonian, no efficient ways to solve the CFW have been reported so far.

In this Letter, in order to address the above problem, we propose the nonequilibrium Green's function's approach to the calculation of the CFW. Based on the Schwinger-Keldysh formalism [28,29], nonequilibrium Green's functions provide a useful framework to handle problems of time-dependent Hamiltonians. For example, it is a standard tool in deriving the Landauer formula in quantum transport [30]. Also, it has been applied to the calculation of the full counting statistics of heat [31]. Inspired by this formalism, we propose the contour for work statistics and define the work functional along the modified contour. In this way, we are able to calculate the CFW of an arbitrary system for a perturbative protocol by the perturbation expansion. Also, to the second order of the expansion, we obtain the general expression of the CFW and demonstrate the fluctuation theorems by utilizing the Kubo-Martin-Schwinger condition [28].

We also notice that Refs. [32,33] discussed the work statistics and fluctuation theorems based on the Schwinger-Keldysh formalism. Different from our modified contour

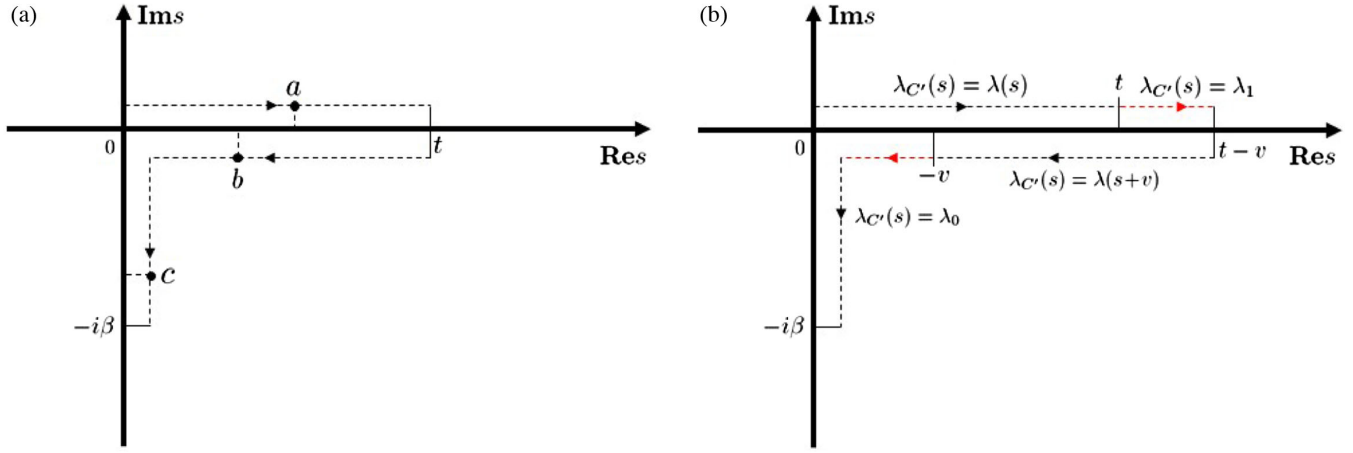


FIG. 1. Complex plane of time s . (a) The Schwinger-Keldysh contour C . Contour ordering: $a < b < c$. (b) The contour for work statistics C' [$\lambda_{C'}(s) = \lambda_0$ in the last two branches]. The red lines denote the exponential operators in Eq. (1). We have assumed $v < 0$ in (b), which does not influence the calculation of the CFW.

for work statistics, they defined the modified Hamiltonian on the usual Schwinger-Keldysh contour. In contrast to their method, where the explicit expression of the modified Hamiltonian is usually difficult to obtain, the correlation functions in our Letter (see below) can be more readily calculated, which significantly simplifies the calculation of the CFW.

From the Schwinger-Keldysh contour to the contour for work statistics.—For a time-dependent quantum system $\hat{H}(s) = \hat{H}_0 + \lambda(s)\hat{H}_1$, $s \in [0, t]$ with the work parameter $\lambda(s)$ and the canonical initial state $\hat{\rho} = e^{-\beta\hat{H}(0)}/\text{Tr}[e^{-\beta\hat{H}(0)}]$ [$\beta = (k_B T)^{-1}$ is the inverse temperature], the expectation value of an observable \hat{O} at time t is $\text{Tr}[\hat{\rho}^I(t)\hat{O}^I(t)]$, where the time-dependent operators are in the interaction picture, $\hat{O}^I(t) = e^{(i/\hbar)\hat{H}_0 t}\hat{O}e^{-(i/\hbar)\hat{H}_0 t}$, $\hat{\rho}^I(t) = e^{(i/\hbar)\hat{H}_0 t}\hat{\rho}(t, 0) \times \hat{\rho}\hat{U}(0, t)e^{-(i/\hbar)\hat{H}_0 t}$. In the Schwinger-Keldysh formalism, this quantity is related to a contour with three directed branches, called the Schwinger-Keldysh contour [see Fig. 1(a)]. Thus, the expectation value can be calculated by a contour integral $\text{Tr}[\hat{\rho}^I(t)\hat{O}^I(t)] = \langle \mathcal{T}_C[\hat{O}^I(t)e^{(i/\hbar)\int_C ds\lambda(s)\hat{H}_1^I(s)}] \rangle / \langle \mathcal{T}_C[e^{(i/\hbar)\int_0^{-i\beta} ds\lambda_0\hat{H}_1^I(s)}] \rangle$,

where $\langle \cdot \rangle = \text{Tr}[e^{-\beta\hat{H}_0}]/\text{Tr}[e^{-\beta\hat{H}_0}]$, the integral is along the contour C , and \mathcal{T}_C indicates ordering along the same contour [e.g., $a < b < c$ in Fig. 1(a)] [28,29].

Inspired by this formalism, we treat both the time-evolution operators and the exponential operators in Eq. (1) as the directed branches of a modified contour C' [see Fig. 1(b)]. Then the contour-integral formulation of the CFW reads

$$\chi(v) = \frac{\langle \mathcal{T}_{C'}[e^{-\frac{i}{\hbar}\int_{C'} ds\lambda_{C'}(s)\hat{H}_1^I(s)}] \rangle}{\langle \mathcal{T}_{C'}[e^{-\frac{i}{\hbar}\int_0^{-i\beta} ds\lambda_0\hat{H}_1^I(s)}] \rangle}, \quad (2)$$

where the integral, the time-ordered operator $\mathcal{T}_{C'}$ and the work parameter $\lambda_{C'}(t)$ are all along the new contour C' . Hence, we call the new contour C' the contour for work statistics, which is also consistent with the Ramsey interferometry [34] and the work statistics in the path integral formalism [35]. Moreover, Eq. (2) can be rewritten as follows:

$$\chi(v) = \frac{\langle \mathcal{T}_{C'}[e^{(i/\hbar)\int_0^t ds\int_0^{hv} dr\dot{\lambda}(s)\hat{H}_1^I(s-r)}] \mathcal{T}_{C'}[e^{-(i/\hbar)\int_0^{-i\beta} ds\lambda_0\hat{H}_1^I(s)}] \rangle}{\langle \mathcal{T}_{C'}[e^{-\frac{i}{\hbar}\int_0^{-i\beta} ds\lambda_0\hat{H}_1^I(s)}] \rangle} \equiv \langle \mathcal{T}_{C'}[e^{i v \hat{W}}] \rangle', \quad (3)$$

where $\dot{\lambda}(s) = d\lambda(s)/ds$ and $\langle \cdot \rangle' = \text{Tr}\{\mathcal{T}_{C'}[e^{-(i/\hbar)\int_0^{-i\beta} ds\lambda_0\hat{H}_1^I(s)}]\} / \text{Tr}\{\mathcal{T}_{C'}[e^{-(i/\hbar)\int_0^{-i\beta} ds\lambda_0\hat{H}_1^I(s)}]\}$. Here, we call $\hat{W} = (1/\hbar v)\int_0^t ds\int_0^{hv} dr\dot{\lambda}(s)\hat{H}_1^I(s-r)$ the work functional (similar to the work functional defined in Ref. [35]). In the classical limit ($\hbar \rightarrow 0$), the time-ordered operator $\mathcal{T}_{C'}$ disappears and the work functional \hat{W} just corresponds to the classical trajectory work $W[x(s), p(s)] = \int_0^t ds\dot{\lambda}(s)H_1(x(s), p(s), s)$ [36]. However, this does not mean that work is an observable [11]. Actually, the work functional \hat{W} is the combination of the operators in different branches of C' . Hence, it is nonsense to consider the eigenstates or eigenvalues of \hat{W} due to $\mathcal{T}_{C'}$.

Calculating work statistics based on the perturbation expansion.—The exponential operator in Eq. (2) can be expanded as

$$\chi(v) = \frac{1 + \sum_{n=1}^{\infty} (\prod_{l=1}^n \int_{C'} d\bar{s}_l) G(s_1, \dots, s_n)}{1 + \sum_{n=1}^{\infty} (\prod_{l=1}^n \int_0^{-i\hbar\beta} d\bar{s}_l) G(s_1, \dots, s_n)}, \quad (4)$$

where $d\bar{s}_l = ds_l \lambda_{C'}(s_l) \theta_{C'}(s_l - s_{l+1})$ is an abbreviation,

$$G(s_1, \dots, s_n) = \left(\frac{-i}{\hbar}\right)^n \langle \hat{H}_1^l(s_1) \cdots \hat{H}_1^l(s_n) \rangle \quad (5)$$

is the n -point correlation function, $\theta_{C'}(s - s')$ is the contour step function [28], and we set $\theta_{C'}(s_n - s_{n+1}) \equiv 1$. A more convenient notion is the series of the logarithm of $\chi(v)$, called the cumulant CFW (see Supplemental Material [37]),

$$\ln \chi(v) = \sum_{n=1}^{\infty} \left(\prod_{l=1}^n \int_{C'} d\bar{s}_l - \prod_{l=1}^n \int_0^{-i\hbar\beta} d\bar{s}_l \right) G_c(s_1, \dots, s_n), \quad (6)$$

where

$$G_c(s_1, \dots, s_n) = \left(\frac{-i}{\hbar}\right)^n \langle \hat{H}_1^l(s_1) \cdots \hat{H}_1^l(s_n) \rangle_c \quad (7)$$

is the n -point cumulant correlation function (also called Ursell function) [38,39]. For the perturbative driving protocol $\lambda(s)$, Eqs. (4) and (6) are the perturbation expansion of the work statistics. Usually, we are able to calculate the correlation functions by Wick's theorem and Feynman diagrams [40]. Here in $G_c(s_1, \dots, s_n)$, only connected diagrams are included.

After a straightforward calculation (see Supplemental Material [37]), to the second order of $\lambda(s)$, we obtain the approximate expression of the perturbation expansion of $\ln \chi(v)$ for a perturbative protocol

$$\begin{aligned} \ln \chi(v) = & iv(\lambda_1 - \lambda_0) \langle \hat{H}_1 \rangle_c + \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{1 - e^{i\omega\hbar v}}{\omega^2} A(\omega) G_c^>(\omega) \\ & + i\hbar v(\lambda_1^2 - \lambda_0^2) \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{G_c^>(\omega)}{\omega} + O[\lambda(s)^3]. \end{aligned} \quad (8)$$

Here, the first term on the rhs of Eq. (8) represents the average work done to the first order of $\lambda(s)$. The second term is called the ‘‘speed’’ term, since $A(\omega)$ depends on $\dot{\lambda}(s)$ by

$$A(\omega) = \left| \int_0^t ds \dot{\lambda}(s) e^{i\omega s} \right|^2. \quad (9)$$

It encodes the information about the nonequilibrium protocols $\lambda(s)$. The third term is called the ‘‘boundary’’ term,

since only the initial and the final value of $\lambda(s)$ appear in this term. Meanwhile, the information about the Hamiltonians \hat{H}_0 and \hat{H}_1 is encoded in the cumulant greater correlation function $G_c^>(\omega)$

$$\begin{aligned} G_c^>(\omega) &= \int_{-\infty}^{\infty} ds G_c^>(s) e^{i\omega s}, \\ G_c^>(s) &= \left(\frac{-i}{\hbar}\right)^2 \langle \hat{H}_1^l(s) \hat{H}_1^l(0) \rangle_c. \end{aligned} \quad (10)$$

We would like to emphasize that Eq. (8) is one of the main results in our Letter. It is a general result of the work statistics because it is valid for arbitrary \hat{H}_0 and \hat{H}_1 , and also arbitrary perturbative protocols $\lambda(s)$.

In the following, we analyze the properties of the CFW based on our results [Eq. (8)]. Above all, the CFW satisfies the normalization condition [$\ln \chi(0) = 0$]. As for the fluctuation theorems, let us first introduce the backward process of $\hat{H}(s)$: $\hat{H}_B(s) = \hat{H}_0 + \lambda(t-s)\hat{H}_1$, $\hat{\rho}_B = e^{-\beta\hat{H}_B(0)}/\text{Tr}[e^{-\beta\hat{H}_B(0)}]$ [41]. Then, the perturbation expansion of $\ln \chi_B(v)$ to the second order of $\lambda(s)$ can be written as

$$\begin{aligned} \ln \chi_B(v) = & -iv(\lambda_1 - \lambda_0) \langle \hat{H}_1 \rangle_c \\ & + \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{1 - e^{i\omega\hbar v}}{\omega^2} A(\omega) G_c^>(\omega) \\ & - i\hbar v(\lambda_1^2 - \lambda_0^2) \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{G_c^>(\omega)}{\omega} + O[\lambda(s)^3]. \end{aligned} \quad (11)$$

Thus, according to the Kubo-Martin-Schwinger condition [28], $G_c^>(s - i\hbar\beta) = G_c^>(-s)$, $e^{-\beta\hbar\omega} G_c^>(\omega) = G_c^>(-\omega)$, and $A(\omega)$ is an even function, from Eqs. (8) and (11) we obtain the following relation:

$$\begin{aligned} -k_B T \ln \frac{\chi(-v + i\beta)}{\chi_B(v)} = & (\lambda_1 - \lambda_0) \langle \hat{H}_1 \rangle_c + \hbar(\lambda_1^2 - \lambda_0^2) \\ & \times \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{G_c^>(\omega)}{\omega} + O[\lambda(s)^3], \end{aligned} \quad (12)$$

where the first and second terms on the rhs of Eq. (12) are exactly the perturbation expansion of the free energy difference $\Delta F = F_{\lambda_1} - F_{\lambda_0} = -k_B T \ln[\text{Tr}(e^{-\beta\hat{H}(t)})/\text{Tr}(e^{-\beta\hat{H}(0)})]$ to the first and the second order of $\lambda(s)$, respectively [38,43]. After taking the inverse Fourier transform of Eq. (12), we obtain the relation between the work distributions of the forward and the backward processes [$P(w)$ and $P_B(w)$] to the second order of $\lambda(s)$

$$\frac{P(w)}{P_B(-w)} = e^{\beta(w - \Delta F)} + O[\lambda(s)^3], \quad (13)$$

which is nothing but the Crooks fluctuation theorem [42,44] to the second-order perturbation expansion of $\lambda(s)$. As a result, the Jarzynski equality [36] to the second-order perturbation expansion can be obtained as a straightforward corollary of Eq. (13) [2].

Example: Noninteracting identical particles in a forced harmonic potential.—To calculate the CFW of a quantum many-body system in an arbitrary nonequilibrium process is an extremely cumbersome task. However, for those perturbative driving protocols, our method based on the nonequilibrium Green's function provides a unified and powerful tool to solve this long-standing problem. We demonstrate our results by considering the following time-dependent Hamiltonian:

$$\begin{aligned}\hat{H}_0 &= \sum_{i=1}^N \frac{\hat{p}_i^2}{2m} + \frac{m}{2} (\omega_x^2 \hat{x}_i^2 + \omega_y^2 \hat{y}_i^2 + \omega_z^2 \hat{z}_i^2), \\ \hat{H}_1 &= \omega_z \sqrt{2m} \sum_{i=1}^N \hat{z}_i,\end{aligned}\quad (14)$$

which describes noninteracting spinless identical particles in a three-dimensional harmonic potential driven along the z direction with the particle mass m , the total particle number N , and the frequencies along three directions ω_x , ω_y , and ω_z . For simplicity, we choose $\omega_x \sim \omega_y \sim \omega_z$. This system is a well-known physical model in statistical physics (e.g., see Ref. [45]). For bosons, it is a good model to study Bose-Einstein condensation in noninteracting trapped gases [45,46]. The transition temperature $k_B T_c$ equals $\hbar \omega_g [N/\zeta(3)]^{1/3}$, where $\omega_g = (\omega_x \omega_y \omega_z)^{1/3}$ and $\zeta(s)$ is the Riemann zeta function. Moreover, the proper thermodynamic limit for these systems is obtained by letting $N \rightarrow \infty$ and $\omega_g \rightarrow 0$, while keeping the product $N \omega_g^3$ as a constant. We would like to emphasize that $\lambda(s)$ does not depend on N . As a result, for various N and the same $\lambda(s)$, we always have $\Delta F/F_{\lambda=0} \sim O(N^0)$ for the canonical ensemble.

After the second quantization, \hat{H}_0 and \hat{H}_1 read

$$\begin{aligned}\hat{H}_0 &= \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}}, \\ \hat{H}_1 &= \sqrt{\hbar \omega_z} \sum_{\mathbf{k}} \sqrt{k_z + 1} (\hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\tilde{\mathbf{k}}} + \hat{a}_{\tilde{\mathbf{k}}}^\dagger \hat{a}_{\mathbf{k}}),\end{aligned}\quad (15)$$

where $\mathbf{k} = (k_x, k_y, k_z) \in \mathbb{N}^3$, $\tilde{\mathbf{k}} = (k_x, k_y, k_z + 1)$, and $\varepsilon_{\mathbf{k}} = \hbar(k_x \omega_x + k_y \omega_y + k_z \omega_z) + \varepsilon_0$ is the single-particle-state energy, $\varepsilon_0 = \hbar(\omega_x + \omega_y + \omega_z)/2$. For later convenience, let us introduce the following notations: The total particle number operator $\hat{N} = \sum_{\mathbf{k}} \hat{n}_{\mathbf{k}} = \sum_{\mathbf{k}} \hat{a}_{\mathbf{k}}^\dagger \hat{a}_{\mathbf{k}}$ with its eigenstates $|\{n_{\mathbf{k}}\}\rangle = \otimes_{\mathbf{k}} |n_{\mathbf{k}}\rangle$; for the canonical ensemble, the density matrix $\hat{\rho}_N = \delta(\hat{N} - N) e^{-\beta \hat{H}_0} / Z_N$,

where $Z_N = \text{Tr}[\delta(\hat{N} - N) e^{-\beta \hat{H}_0}]$, $\langle \{n_{\mathbf{k}}\} | \delta(\hat{N} - N) | \{n'_{\mathbf{k}}\} \rangle = \delta_{\{n_{\mathbf{k}}\}, \{n'_{\mathbf{k}}\}} \delta_{N, \sum_{\mathbf{k}} n_{\mathbf{k}}}$. Here $\delta_{\cdot, \cdot}$ is the Kronecker delta function; the mean occupation number in the canonical ensemble $\bar{n}_{\mathbf{k}}(N) = \text{Tr}[\hat{\rho}_N \hat{n}_{\mathbf{k}}]$; for the grand canonical ensemble, the density matrix $\hat{\rho}_\mu = e^{-\beta(\hat{H}_0 - \mu \hat{N})} / Z_\mu$, where $Z_\mu = \text{Tr}[e^{-\beta(\hat{H}_0 - \mu \hat{N})}] = \prod_{\mathbf{k}} (1 - \gamma \alpha e^{-\beta \varepsilon_{\mathbf{k}}})^{-\gamma}$, $\gamma = 1, -1$ for bosons and fermions, respectively; the fugacity $\alpha = e^{\beta \mu}$; the mean occupation number in the grand canonical ensemble $\bar{n}_{\mathbf{k}}(\mu) = \text{Tr}[\hat{\rho}_\mu \hat{n}_{\mathbf{k}}] = 1/[e^{\beta(\varepsilon_{\mathbf{k}} - \mu)} - \gamma]$. In addition, quantities in these two ensembles are related by the fugacity expansions [45]

$$\begin{aligned}Z_\mu &= 1 + \sum_{N=1}^{\infty} \alpha^N Z_N, \\ Z_\mu \bar{n}_{\mathbf{k}}(\mu) &= \sum_{N=1}^{\infty} \alpha^N Z_N \bar{n}_{\mathbf{k}}(N).\end{aligned}\quad (16)$$

Similarly, we obtain the relation between the characteristic functions of work in these two ensembles

$$Z_\mu \chi_\mu(v) = 1 + \sum_{N=1}^{\infty} \alpha^N Z_N \chi_N(v).\quad (17)$$

Thus, according to Eq. (10) and Wick's theorem in the grand canonical ensemble, we obtain the cumulant greater correlation function in the grand canonical ensemble

$$\begin{aligned}G_\mu^>(\omega) &= -\frac{2\pi\omega_z}{\hbar} \sum_{\mathbf{k}} (k_z + 1) \{ \delta(\omega - \omega_z) \\ &\quad \times [\bar{n}_{\mathbf{k}}(\mu) + \gamma \bar{n}_{\mathbf{k}}(\mu) \bar{n}_{\tilde{\mathbf{k}}}(\mu)] \\ &\quad + \delta(\omega + \omega_z) [\bar{n}_{\tilde{\mathbf{k}}}(\mu) + \gamma \bar{n}_{\mathbf{k}}(\mu) \bar{n}_{\tilde{\mathbf{k}}}(\mu)] \}.\end{aligned}\quad (18)$$

Then from Eqs. (16) and (18), we obtain the cumulant greater correlation function in the canonical ensemble

$$\begin{aligned}G_N^>(\omega) &= -\frac{2\pi\omega_z}{\hbar} \sum_{\mathbf{k}} (k_z + 1) \{ \delta(\omega - \omega_z) [\bar{n}_{\mathbf{k}}(N) + \gamma \xi_{\mathbf{k}}(N)] \\ &\quad + \delta(\omega + \omega_z) [\bar{n}_{\tilde{\mathbf{k}}}(N) + \gamma \xi_{\tilde{\mathbf{k}}}(N)] \},\end{aligned}\quad (19)$$

where we have defined $\xi_{\mathbf{k}}(N)$ as

$$Z_\mu \bar{n}_{\mathbf{k}}(\mu) \bar{n}_{\tilde{\mathbf{k}}}(\mu) = \sum_{N=1}^{\infty} \alpha^N Z_N \xi_{\mathbf{k}}(N).\quad (20)$$

Finally, substituting Eqs. (18) and (19) in Eq. (8) and considering $\langle \hat{H}_1 \rangle_c = 0$, we obtain the perturbation expansion of the cumulant CFW to the second order of $\lambda(s)$ with the canonical and the grand canonical initial state, respectively,

$$\ln \chi_N(v) \approx -4 \sum_{\mathbf{k}} [\gamma(k_z + 1) \xi_{\mathbf{k}}(N) + k_z \bar{n}_{\mathbf{k}}(N)] \frac{\sin^2(v \hbar \omega_z / 2)}{\hbar \omega_z} A(\omega_z) + N \left(-iv(\lambda_1^2 - \lambda_0^2) + \frac{e^{iv\hbar\omega_z} - 1}{\hbar \omega_z} A(\omega_z) \right), \quad (21)$$

$$\ln \chi_{\mu}(v) \approx -4 \sum_{\mathbf{k}} [\gamma(k_z + 1) \bar{n}_{\mathbf{k}}(\mu) \bar{n}_{\bar{\mathbf{k}}}(\mu) + k_z \bar{n}_{\mathbf{k}}(\mu)] \frac{\sin^2(v \hbar \omega_z / 2)}{\hbar \omega_z} A(\omega_z) + \bar{N}(\mu) \left(-iv(\lambda_1^2 - \lambda_0^2) + \frac{e^{iv\hbar\omega_z} - 1}{\hbar \omega_z} A(\omega_z) \right), \quad (22)$$

where $\bar{N}(\mu) = \sum_{\mathbf{k}} \bar{n}_{\mathbf{k}}(\mu)$ is the average particle number in the grand canonical ensemble. We would like emphasize that Eqs. (21) and (22) are valid for both bosons and fermions and arbitrary large N , where previous methods fail [47].

Based on the analytical solutions of the CFW [Eqs. (21) and (22)], we study the properties of the work statistics in several special cases:

(1) Single-particle case ($N = 1$): In this case, we have $Z_1 = \sum_{\mathbf{k}} e^{-\beta \epsilon_{\mathbf{k}}} = [8 \sinh(\beta \omega_x / 2) \sinh(\beta \omega_y / 2) \times \sinh(\beta \omega_z / 2)]^{-1}$, $\bar{n}_{\mathbf{k}}(1) = e^{-\beta \epsilon_{\mathbf{k}}} / Z_1$, $\xi_{\mathbf{k}}(1) = 0$ [Eqs. (16) and (20)] and, accordingly,

$$\ln \chi_1(v) = \frac{-4 \sin^2(v \hbar \omega_z / 2)}{\hbar \omega_z (e^{\beta \hbar \omega_z} - 1)} A(\omega_z) - iv(\lambda_1^2 - \lambda_0^2) + \frac{e^{iv\hbar\omega_z} - 1}{\hbar \omega_z} A(\omega_z). \quad (23)$$

Actually, Eq. (23) is identical to the exact expression of the cumulant CFW in Ref. [17], which indicates that, for $N = 1$, the contributions from the third or higher orders of $\lambda(s)$ vanish (see the Supplemental Material [37]).

(2) Nondegenerate case (in the thermodynamic limit $\epsilon_0 \sim \hbar \omega_z \sim N^{-1/3}$ and $k_B T \gg N^{1/3} \hbar \omega_g$): From Eq. (23), we obtain the classical limit of the cumulant CFW for a single particle [48]

$$\ln \chi_1^{\text{CL}}(v) = -v^2 k_B T A(\omega_z) - iv[\lambda_1^2 - \lambda_0^2 - A(\omega_z)]. \quad (24)$$

In the nondegenerate case, we have $Z_1 \approx (k_B T)^3 / (\hbar \omega_g)^3$, which is equal to the partition function of a classical harmonic oscillator, $Z_N = Z_1^N / N!$, $Z_{\mu} = e^{\alpha Z_1}$, $\bar{n}_{\mathbf{k}}(N) = N e^{-\beta \epsilon_{\mathbf{k}}} / Z_1$, $\bar{n}_{\mathbf{k}}(\mu) = \alpha e^{-\beta \epsilon_{\mathbf{k}}}$, $\bar{n}_{\mathbf{k}}(\mu) \bar{n}_{\bar{\mathbf{k}}}(\mu) \ll \bar{n}_{\mathbf{k}}(\mu)$, $\xi_{\mathbf{k}}(N) \ll \bar{n}_{\mathbf{k}}(N)$ (dilute gas). From Eqs. (21) and (22), we obtain the cumulant characteristic functions of work for many particles in two ensembles

$$\ln \chi_N^{\text{CL}}(v) = N \ln \chi_1^{\text{CL}}(v), \quad \ln \chi_{\mu}^{\text{CL}}(v) = \alpha Z_1 \ln \chi_1^{\text{CL}}(v), \quad (25)$$

which indicates that the particles satisfy Maxwell-Boltzmann statistics and the contributions from the third or higher orders of $\lambda(s)$ vanish.

The discussions about the CFW in the degenerate case are shown in the Supplemental Material [37].

Summary.—The CFW is an important quantity to characterize the nonequilibrium process of the time-dependent quantum systems, especially of quantum many-body systems. But the calculation of the CFW for quantum many-body systems has been a long-time conundrum. To overcome this difficulty, by utilizing the nonequilibrium Green's function's method, we formulate the work statistics with a contour integral and obtain the series expansion of the CFW. This method is valid for arbitrary \hat{H}_0 and \hat{H}_1 , as well as for arbitrary perturbative work protocols $\lambda(s)$. Hence, it provides a unified method for the calculation of the CFW. In this framework, work, although not an observable, is defined as a functional along the modified contour. To the second order of the work parameter, the CFW is expressed as the sum of the first-order term, the speed term, and the boundary term. Moreover, the fluctuation theorems can be demonstrated by utilizing the Kubo-Martin-Schwinger condition. As an example, we calculate the CFW of noninteracting identical particles in a forced harmonic potential, where previous methods fail. In the future, we expect to investigate the effects of relativity and interactions with our methods.

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