Sum rule for fluctuations of work

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We study the fluctuations of work caused by applying cyclic perturbations and obtain an exact sum rule satisfied by the moments of work for a broad class of quantum stationary ensembles. In the case of the canonical ensemble, the sum rule reproduces the Jarzynski equality. The sum rule can also be simplified into a linear relationship between the work average and the second moment of work, which we numerically confirm via an exact diagonalization of a spin model system.

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I. INTRODUCTION

Under cyclic variation of a system parameter, a system will generally proceed to a different state from its initial state. The energy change that occurs accordingly amounts to work W done on the system if the system is isolated. This work is a random quantity for small systems, and their distribution depends on all details of the force protocol, such as its duration and strength, as well as the system's initial state. So-called fluctuation relations for classical or quantum systems have attracted much attention in recent decades [1–4]. The class of systems for which one knows such fluctuation relation is mainly restricted to systems in a canonical [5,6] or in a grand canonical initial state [7]. There are two types of fluctuation relations, the detailed ones also known as Crooks relations and the integral relations known as Jarzynski equalities. Crooks relations also extend to systems in a microcanonical initial state [8–11], while the rigorous derivation of the Jarzynski equality requires a canonical or grand canonical initial state.

Meanwhile, for weak cyclic force protocols acting on a system in a microcanonical initial state at the energy E, another type of fluctuation relation was derived in Ref. [12]. It connects the first two moments of work as

$$W_1(E) \approx \frac{1}{2\omega(E)} \frac{\partial \omega(E)}{\partial E} W_2(E), \tag{1}$$

where W_1 and W_2 are the work average and the second moment of work, respectively. This relation is particularly significant in the aspect that it predicts the universal form of the energy distribution of nonequilibrium states reached after many cyclic processes [12]. The crucial assumptions in the derivation of this relation are that the density of states, $\omega(E)$, and the moments of work are smooth functions of the energy E and that the work is approximately Gaussian distributed. However, how we can reconcile those assumptions with the frequent observations that the work statistics of quantum systems typically are non-Gaussian [13] and moreover that quantum systems have discrete spectra [13] remains a question.

In the present study, we scrutinize the work fluctuations caused by a cyclic force protocol and examine the validity of the relation (1). We first derive an exact sum rule (10) that governs the relation between the work average and the higher moments of work, which is valid for a broad class of quantum stationary ensembles as initial states. In this ensemble class, the occupation probability of an energy eigenstate is determined by a continuous and differentiable function. If this function is taken to be exponential, a canonical ensemble is recovered, and then the sum rule reproduces the Jarzynski equality. On the other hand, upon choosing the function to have a narrow width, the corresponding initial ensemble simulates a smoothed version of a quantum microcanonical ensemble, which is advantageous for dealing with some technical difficulties posed by the discrete nature of quantum systems. With the exact sum rule, we show that a linear relation between the first two moments of work can exist in a form similar to (1) but with a different proportionality coefficient. We also specify the conditions to obtain the linear relation and point out that the Gaussianity of work distribution is not essential. Finally, via exact enumeration of eigenvalues and eigenstates of a spin model system, we numerically investigate the validity of the linear relationship in the case of the smoothed microcanonical initial state.

This paper is organized as follows: Sec. II introduces the initial ensembles in which the energy eigenstates of an initial Hamiltonian are populated following smooth functions. We also recollect the definition of work for quantum systems, the probability of observing work values, and the corresponding expressions of work moments. In Sec. III we derive an exact sum rule that governs the work moments. We discuss Jarzynski equality as a particular form of the sum rule. Also, we deduce a linear relationship akin to Eq. (1) from the sum rule. We show therein that, instead of the density of states $\omega(E)$, a smooth function of E related to the normalization factor of the initial ensemble determines the proportional constant. In the subsequent Sec. IV, we take a model system of spins (the Heisenberg XXX model in one dimension), considering

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a weak and local perturbation as a force protocol. We demonstrate that work moments in the considered setting satisfy the linear relationship. Finally, Sec. V summarizes our study.

II. INGREDIENTS

We first describe the basic elements of our study, the initial ensembles, work, and its probability for quantum systems.

A. Initial ensembles

As initial states to which a perturbation shall be applied, we consider a stationary ensemble of the unperturbed Hamiltonian $\hat{H}_0$, which is defined for any energy by means of a diagonal density matrix in the eigenbasis of $\hat{H}_0$:

$$\hat{\rho}(E) = \frac{1}{D(E)} \sum_i m_i(E) \hat{\Pi}_i, \tag{2}$$

where $\hat{\Pi}_i$ denotes the ith eigenprojector of $\hat{H}_0$, hence, $\hat{H}_0 = \sum_i E_i \hat{\Pi}_i$ with E_i being the ith eigenvalue, obeying $\hat{\Pi}_i \hat{\Pi}_j = \delta_{i,j} \hat{\Pi}_i$ and $\sum_i \hat{\Pi}_i = \mathbb{1}$. $D(E)$ in Eq. (2) is the normalization factor given by

$$D(E) = \sum_i m_i(E) \mathrm{Tr} \hat{\Pi}_i. \tag{3}$$

The weights $m_i(E)$ are smooth functions determined by a single, smooth master function $m(x)$ according to $m_i(E) = m[(E - E_i)/\epsilon]$, where $\epsilon > 0$ is an energy scale.

The formula (2) has two properties: First, it is diagonal in the energy basis, and, second, it determines the occurrence of an energy eigenstate having energy E by a single-argument function $m(x)$. The first property applies to the equilibrium ensembles. Also, it applies to any ensembles acquired immediately after performing the ideal von Neumann projective energy measurement. Since work in a quantum system is defined as the difference between energies at the beginning and the end of a work protocol, the energy measurement at the protocol beginning is necessary and naturally comes in. So the first property fits generally the purpose of investigating work done by quantum systems. The assumption of the single-argument function has no proof that this is always the case. However, the equilibrium ensembles are well presented by the single-argument functions, and the very common Gaussian weight [14–17] is also determined by the single argument. Thus, we believe that the single-argument assumption is not very restrictive. We also show in Appendix A that the canonical ensemble can be derived from the reduced density matrix for a small subsystem of a total system described by Eq. (2).

Specifically, when choosing the expression for the master function to be

$$m(x) = \frac{2}{1 + \cosh(x)}, \tag{4}$$

we can simulate the microcanonical ensemble in the limit of very small ϵ because the resulting smoothing functions $m_i(E)$ reach their maximal values at $E = E_i$ and become vanishingly small for E_i located from E such that $|E - E_i| \gg \epsilon$. When choosing $m(x) = \Theta(x + 1) - \Theta(x - 1)$ with $\Theta(x)$ being the Heaviside step function, Eq. (2) corresponds to the microcanonical ensemble of energy eigenstates that falls within an energy shell of width 2ϵ centered at E [18–20].

Another strict definition of the microcanonical ensemble of $\hat{H}_0$ reads [9,11,21,22]

$$\hat{\rho}_{E_i} = \frac{\hat{\Pi}_i}{D_{E_i}}, \tag{5}$$

where the normalization factor D_{E_i} is given by the degeneracy of the ith energy eigenvalue as $D_{E_i} = \mathrm{Tr}\hat{\Pi}_i$. The microcanonical ensemble density matrix defined in this way only on the subset of eigenstates having the specific energy value renders its use rather cumbersome in many cases. For instance, the density of states $\omega(E)$ that enters Eq. (1) is given by the sum of the delta functions,

$$\omega(E) = \sum_i \delta(E - E_i) D_{E_i}. \tag{6}$$

This is a highly singular function tricky to handle, requiring a smoothing scheme for its computation [23,24]. On the other hand, Eq. (3) resembles Eq. (6) in the limit of very small ϵ, its analytic property allows a more tractable approach.

In passing, we note that the master function $m(x)$ is not restricted to the form of Eq. (4). Rather, any positive master function $m(x)$ generates a density matrix describing a stationary ensemble provided that the normalizing factor $D(E)$ exists. The latter condition is always satisfied for systems with a finite dimensional Hilbert space. In particular, the exponential master function $m(x) = e^x$ generates the E-independent canonical density matrix $\rho_c = Z_\beta^{-1} e^{-\beta \hat{H}_0}$ with $Z_\beta = \mathrm{Tr} e^{-\beta \hat{H}_0}$, where the inverse temperature β is given by the energy scale ϵ. The normalization factor becomes $D(E) = e^{\beta E} Z_\beta$. We see later that in the case of the exponential master function, our sum rule for work moments becomes Jarzynski equality.

B. Work and its probability

The work applied to a system by the external variation of some of its parameters according to a force protocol is defined as the difference between the system's energies at the end and the beginning of the protocol. For a quantum system, these energies ideally are the results of projective measurements of the instantaneous Hamiltonians at the respective times. For cyclic protocols, these Hamiltonians agree with each other. Hence, the possible work values are given by the differences of a pair of energy eigenvalues of $\hat{H}_0$, that is, $W = E_j - E_i$ where E_i is the result of the measurement just before the beginning of the force protocol and E_j is that of the one immediately after the end of the force protocol.

The joint probability of measuring E_i and subsequently E_j results as

$$p_{j,i} = \mathrm{Tr} \hat{\Pi}_j \hat{U} \hat{\Pi}_i \hat{\rho}(E) \hat{U}^\dagger, \tag{7}$$

where $\hat{U}$ is the time evolution operator and $\hat{\rho}(E)$ is the density matrix of the initial state given by Eq. (2). This joint probability determines the probability of work, given by the following expression:

$$P_W(E) = D(E)^{-1} \sum_{i,j} \delta_{W, E_j - E_i} m_i(E) \mathrm{Tr} \hat{\Pi}_j \hat{U} \hat{\Pi}_i \hat{U}^\dagger. \tag{8}$$

The moments of work are accordingly given by

$$W_n(E) = \sum_W W^n P_W(E), \quad n = 1, 2, \ldots. \tag{9}$$

We are now ready to establish an exact relation between these work moments.

III. AN EXACT SUM RULE FOR WORK FLUCTUATION

The main result of the present study is that for all smooth stationary ensembles as given by Eq. (2) the moments of work satisfy an exact sum rule:

$$W_1(E) = \frac{1}{D(E)} \sum_{n=2} \frac{(-1)^n}{n!} \frac{d^{n-1}}{dE^{n-1}} [D(E) W_n(E)]. \tag{10}$$

The proof of this relation begins with a formal identity:

$$\sum_W \sum_{i,j} \delta_{W,E_j-E_i} F\left(\frac{E-W-E_i}{\epsilon}\right) \mathrm{Tr}\hat{\Pi}_j \hat{U} \hat{\Pi}_i \hat{U}^\dagger$$
$$= \sum_W \sum_{i,j} \delta_{W,E_j-E_i} F\left(\frac{E-E_j}{\epsilon}\right) \mathrm{Tr}\hat{\Pi}_j \hat{U} \hat{\Pi}_i \hat{U}^\dagger, \tag{11}$$

where $F(x)$ is an incomplete integral of the master function $m(x)$. By assumption, $m(x)$ is infinitely many times differentiable everywhere, so is $F(x)$. The first derivative of $F(x)$ agrees with $m(x)$,

$$m_i(E) = \left[\frac{dF(x)}{dx}\right]_{x=(E-E_i)/\epsilon}. \tag{12}$$

As the next step, we expand the function $F((E-W-E_i)/\epsilon)$ on the left-hand side of (11) as a power series of W to get

$$F\left(\frac{E-W-E_i}{\epsilon}\right) = \sum_{n=0}^{\infty} \frac{(-W)^n}{\epsilon^n n!} \left.\frac{d^n F(x)}{dx^n}\right|_{x=\frac{E-E_i}{\epsilon}}. \tag{13}$$

Upon this substitution, the contribution from the zeroth order in W on the left-hand side of Eq. (11) cancels the right-hand side of Eq. (11) due to the time-reversal symmetry $\mathrm{Tr}\hat{\Pi}_j \hat{U} \hat{\Pi}_i \hat{U}^\dagger = \mathrm{Tr}\hat{\Pi}_i \hat{U} \hat{\Pi}_j \hat{U}^\dagger$ so that we obtain

$$\sum_{n=1} \frac{1}{n!} \frac{d^{n-1}}{dE^{n-1}} \sum_W (-W)^n$$
$$\times \left[\sum_{i,j} \delta_{W,E_j-E_i} m_i(E) \mathrm{Tr}\hat{\Pi}_j \hat{U} \hat{\Pi}_i \hat{U}^\dagger\right] = 0. \tag{14}$$

Recalling the expression of work probability, Eq. (8), we can identify the terms in the square brackets by $D(E)P_W(E)$. Using the definition of the nth moment of work (9), the summation over W leads the above infinite series to the sum rule given in Eq. (10). Although it is an exact relation for the large class of stationary states where the master function is expressed only in terms of a constant-shifted variable with a overall scale factor, i.e., $x = (E-E_i)/\epsilon$ as in Eq. (14), this sum rule may yet appear rather unwieldily due to the presence of moments (cumulants) and their derivatives up to arbitrarily high orders. In the remainder of this section, we consider a case where the sum rule yields a closed expression and situations where it leads to a handier approximate relation similar to Eq. (1).

A. Jarzynski equality as a special case of Eq. (10)

As mentioned earlier, taking the exponential master function $m(x) = e^x$ leads to a canonical density matrix at the temperature $\epsilon = \beta^{-1}$: Eq. (2) reads as

$$\hat{\rho}(E) = \frac{1}{D(E)} \sum_i e^{\beta(E-E_i)} \hat{\Pi}_i \tag{15}$$
$$= Z_\beta^{-1} \sum_i e^{-\beta E_i} \hat{\Pi}_i. \tag{16}$$

In obtaining the second line, we used the fact that the normalization factor $D(E)$ in the case of the exponential master function is determined as

$$D(E) = e^{\beta E} \sum_i e^{-\beta E_i} \hat{\Pi}_i \equiv e^{\beta E} Z_\beta. \tag{17}$$

This normalization factor of such form presents a relation

$$\frac{d^{n-1} D(E)}{dE^{n-1}} = \beta^{n-1} D(E). \tag{18}$$

Note also that the density matrix (15) is independent of the energy parameter E, and consequently, the probability of work and all moments of work are independent of E. More explicitly, by writing the probability of work from Eq. (8) as

$$P_W(E) = \sum_{i,j} \delta_{W,E_j-E_i} \frac{e^{-\beta E_i}}{Z_\beta} \mathrm{Tr}\hat{\Pi}_j \hat{U} \hat{\Pi}_i \hat{U}^\dagger, \tag{19}$$

one finds that this expression is the work probability for a canonical initial state.

Now using the E independence of work moments and the relation (18) for the derivatives of $D(E)$, we find that Eq. (10) can be written as

$$\sum_{n=1} \frac{(-1)^n}{n!} \beta^n W_n(E) = 0, \tag{20}$$

where the nonzero $D(E)$ is divided and dropped out. Because $\sum_W W^n P_W(E) = W_n$, Eq. (20) is equivalent to

$$\sum_W P_W(E) e^{-\beta W} = 1, \tag{21}$$

which is the Jarzynski equality for the canonical initial states.

B. Approximate fluctuation relation, Eq. (1)

Apart from rare cases allowing an exact treatment, such as seen above in the case of the canonical initial states, the sum rule (10) can be used to find criteria allowing the approximate fluctuation relation (1). For example, if all contributions higher than the second order to the sum are negligible, the approximate fluctuation relation,

$$W_1(E) \approx (1/2)\beta_D(E) W_2(E) + (1/2) dW_2(E)/dE, \tag{22}$$

is obtained. Here an inverse-temperature-like quantity β_D is defined as

$$\beta_D(E) \equiv d \ln D(E)/dE. \tag{23}$$

If, additionally, the energy derivative of the second moment can be neglected, we get

$$W_1(E) \approx \frac{\beta_D(E)}{2} W_2(E), \tag{24}$$

which is almost similar to Eq. (1). Only difference from Eq. (1) is that the appeared proportional factor is not the derivative of the density of states but the normalization factor of the smoothed ensemble (2). A question now is whether those seemingly independent assumptions can be justified in what circumstances. In the next section, considering a weak and local perturbation on a system of Heisenberg XXX spins as a concrete example, we numerically validate this linear relation (24).

Before going over the next section, we would like to point out that even if one assumes a Gaussian distributed work probability as suggested in Ref. [12], one does not get the series (10) terminated. This point can be seen explicitly, using the cumulant generating function of work,

$$\mathcal{C}(\lambda, E) = \ln \sum_W e^{\lambda W} P_W(E), \tag{25}$$

and rewriting Eq. (10) as

$$\sum_{n=1} \frac{(-1)^n}{n!} \frac{d^{n-1}}{dE^{n-1}} \left[D(E) \left(\frac{d^n}{d\lambda^n} e^{\mathcal{C}}(\lambda, E) \right)_{\lambda=0} \right] = 0. \tag{26}$$

When the work probability is Gaussian, the cumulant generating function is given by $\mathcal{C}(\lambda, E) = W_1(E)\lambda + (\lambda^2/2)[W_2(E) - W_1^2(E)]$. Yet we see that the above series still contains the higher order derivatives ($n > 2$). Therefore, the Gaussianity of work distribution appears not to be an essential element for the validity of Eq. (1).

IV. NUMERICAL TEST

Let us now examine Eq. (24) numerically. We take the quantum-spin model in our numerical calculations, the so-called Heisenberg XXX model described by the Hamiltonian,

$$\hat{H}_0 = -\frac{J}{2} \sum_{k=1}^{N} \vec{\sigma}_k \cdot \vec{\sigma}_{k+1}. \tag{27}$$

Here $\vec{\sigma}_k = (\hat{\sigma}_k^x, \hat{\sigma}_k^y, \hat{\sigma}_k^z)$ are the Pauli matrices for a spin-1/2 located at the kth site of one-dimensional lattice having N number of sites in total. We impose the periodic boundary conditions: $\vec{\sigma}_k = \vec{\sigma}_{k+N}$. In this model, spins interact with their nearest neighboring spins, and J measures the interaction strength. We set $J = 1$ and use it as an energy unit in presenting our numerical results.

We consider an initial ensemble of this spin system, choosing the master function in the density matrix (2) to be

$$m_i(E) = \frac{2}{1 + \cosh[(E - E_i)/\epsilon]}. \tag{28}$$

As said, the corresponding density matrix mimics the microcanonical ensemble by the width parameter ϵ chosen small. We fix ϵ to be 1.5 times the maximum level spacing of the Hamiltonian $\hat{H}_0$ for our numerical calculations. In order to check whether the master function with the chosen ϵ well

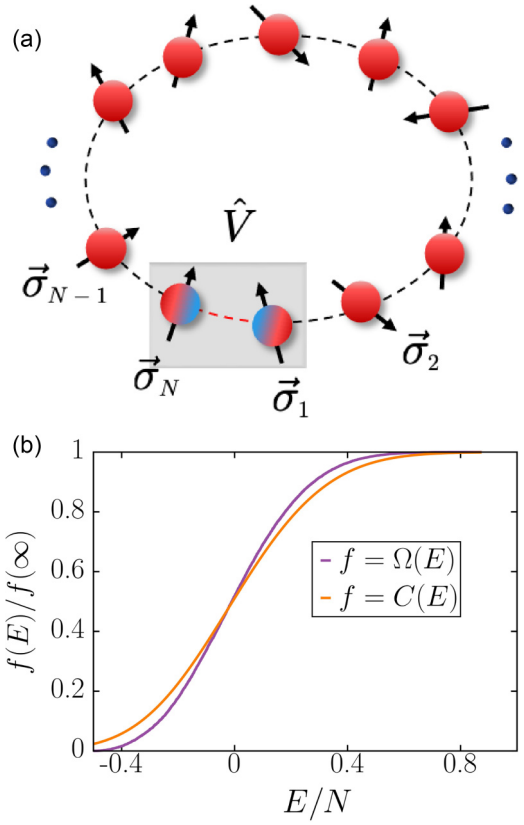

FIG. 1. (a) Schematic picture of the model system used for the numerical test of Eq. (22); the shaded region marks the two spins on which the perturbation (33) acts. (b) Normalized cumulative counting functions, $\Omega(E)/\Omega(\infty)$ defined in Eq. (29). To compare, it also displays $C(E)/C(\infty)$ defined in Eq. (30) and numerically calculated for the spin model system (27).

describes the energy level populations of the considered system, we compare two quantities: One is a cumulative counting function of the number of energy states below the energy E,

$$\Omega(E) = \int_{-\infty}^{E} dE' \omega(E'), \tag{29}$$

which is given by the density of states integrated up to an energy E. Unlike the density of states, a singular function given by the series of delta functions, the cumulative counting $\Omega(E)$ renders an adequate measure for a qualitative comparison. We take the corresponding quantity in the case of the smoothed microcanonical ensemble to compare with $\Omega(E)$ to be

$$C(E) = \int_{-\infty}^{E} dE' D(E'). \tag{30}$$

As shown in Fig. 1, $C(E)$ [normalized by $C(\infty)$] and the accordingly normalized $\Omega(E)$ are in relatively good agreement with each other.

The above-described spin chain is subject to a cyclic perturbation $\hat{V}(t)$ that extends over the period τ. We take the form of quench as a simple time dependence,

$$\hat{V}(t) = \begin{cases} \hat{V} & \text{if } 0 < t < \tau \\ 0 & \text{otherwise.} \end{cases} \tag{31}$$

While this perturbation is in operation, the time evolution operator is given by

$$\hat{U}(\tau) = e^{-i\hat{H}\tau/\hbar}, \quad \hat{H} = \hat{H}_0 + \hat{V}, \tag{32}$$

where $\hat{H}$ denotes the total Hamiltonian during the evolution. We choose the perturbation potential to act only on two spins as

$$\hat{V} = -\lambda \hat{\sigma}_N^z \hat{\sigma}_1^z. \tag{33}$$

This short-range perturbation can be considered weak for moderately small values of λ. In our numerical calculations, we set $\lambda = 0.2$ in the energy unit, J. Upon choosing such weak perturbation, we expect that its yielded work moments W_n are such that their absolute magnitude stays small with increasing order of the moments, and the lower order contributions in the sum rule would possibly be the dominant ones.

In order to calculate the quantities that appear in Eq. (10) and its approximate expression (22) in the setting described above, we adopt the exact diagonalization technique to find the eigenvalues and eigenvectors of the model Hamiltonians (27) [25]. Taking explicitly into account all symmetries of the models, such as symmetry under spin inversion and spatial reflection symmetry for the perturbed systems and additionally translational symmetry for the unperturbed systems, we perform our numerical investigation on the spin chain of length $N = 17$.

A. Confirmation of Eq. (24)

We now numerically demonstrate the validity of the approximate relation (24) between the first moment and the second moment of work. While those moments are functions of τ, the duration of the force protocol, instead of choosing particular values of τ, we consider the long-time averages of the moments determined by

$$\overline{W}_n(E) \equiv \lim_{T\to\infty} \int_0^T d\tau W_n(E). \tag{34}$$

Due to the linearity of the sum rule with respect to the moments, the long-time averages of the work moments W_n obey the identical sum rule. Hereafter, we present our results for these long-time averages.

As we see in Fig. 2(a), the curve of $\overline{W}_1(E)$ versus $\beta_D(E)\overline{W}_2(E)$ is positioned mostly along the straight line, showing that the relation (24) is fairly valid. A noteworthy point here is that because $\overline{W}_2(E)$ is non-negative, the sign of the work average $\overline{W}_1(E)$ is determined by the inverse temperature-like quantity $\beta_D(E)$. Meanwhile, the sign of $\beta_D(E)$ defined in Eq. (23) indicates whether $D(E)$ is an increasing or decreasing function at E. So when the energy factor E of the initial ensemble is at regions where $D(E)$ increases, the average energy of the system increases after the cyclic process of the quench type (31) is applied. The average energy decreases when E of the initial ensemble is located at the $D(E)$-decreasing region. We display the behavior of $\beta_D(E)$ as a function of E/N in Fig. 2(b) [see the curve for $O = D(E)$]. In the case of the spin model used in our calculation, an energy spectrum is bounded below and above. As E increases from the ground state energy, $D(E)$ increases and reaches its maximum at $E \approx 0$. When E increases further, $D(E)$ decreases. This behavior of $D(E)$ explains the sign change of β_D around at $E \approx 0$ in Fig. 2(b). Also, in the same panel, we plot the logarithmic derivative of the long-time-average of the second moment $\overline{W}_2(E)$, in which one can see that its magnitude stays almost zero compared to $\beta_D(E)$. The results explicitly show that the energy derivative of the second moment makes negligible contribution in determining the relation between the first and the second moment of work, as assumed in obtaining the relation, Eq. (24).

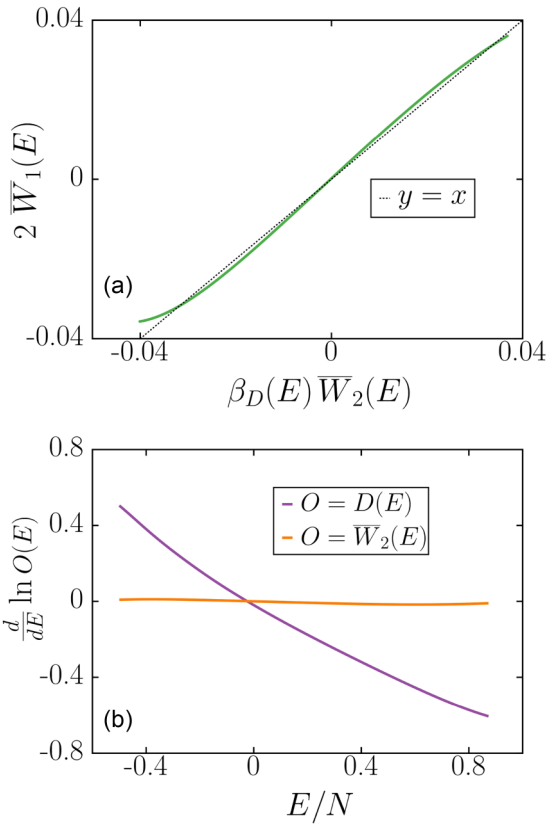

FIG. 2. Numerical test of Eq. (24) for the spin model systems of size $N = 17$. (a) Linear relationship between the two work moments. (b) Logarithmic derivative of $D(E)$ and the second moment.

Now we analyze the higher-order contributions, questioning whether the linear relationship displayed in Fig. 2 is due to the mutual cancellation between terms of the higher order moments or it is due to the smallness of the individual terms. To see the effect of the terms discarded from the exact relation (10) systematically, let us define a finite sum:

$$M^{(n)}(E) = \frac{1}{D(E)} \sum_{k=2}^{n} \frac{(-1)^k}{k!} \frac{d^{k-1}}{dE^{k-1}} [D(E)\overline{W}_k(E)], \tag{35}$$

whereby the sum rule (10) can be read as $\overline{W}_1(E) = M^{(\infty)}(E)$. We omit the function argument E for notation simplicity in the discussion hereafter. Note that Fig. 2(a) displays the relation between the work average $\overline{W}_1$ versus this finite sum up to $n = 2$, $M^{(2)}$. When $n = 3$, $M^{(3)}$ includes the additional contribution from the third-order moment of work. Therefore, the magnitude of the contributions from the nth work moment is estimated from the degree of variation of $M^{(n)}$: $M^{(n)} - M^{(n-1)}$.

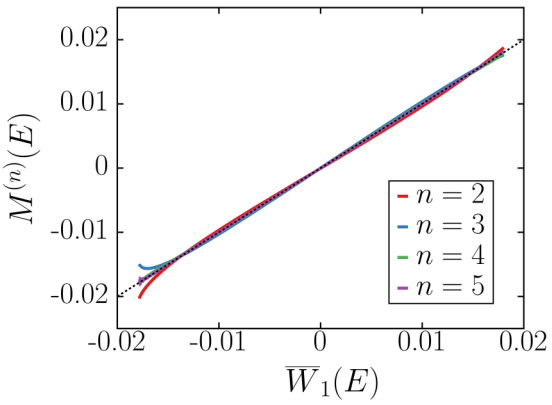

FIG. 3. The finite sum (35) vs work average $\overline{W}_1$. The system size used is $N = 17$. The finite sum for $n \geqslant 3$ is largely the same as that given by $n = 2$.

In Fig. 3 we show $M^{(n)}$ vs $\overline{W}_1$, up to $n = 5$. The $M^{(2)}$ aligned along $y = x$ is the behavior previously illustrated in Fig. 2(a); only the chosen axes are different. Interestingly, $M^{(3)}$ also maintains the linear relationship, suggesting that $d^2[D\overline{W}_3]/dE^2$ makes a negligible contribution to the sum. Including higher order moments such as $n = 4, 5$ does not alter much the behavior of the finite sum, except it provides a better fit to $\overline{W}_1$ close to the left boundary values. From this numerical evidences, one can infer that

$$\frac{d^{k\geqslant 3}}{dE^k}\left[\frac{D\overline{W}_{k+1}}{(k+1)!}\right] \ll \frac{1}{2}\frac{d}{dE}(D\overline{W}_2), \quad D\overline{W}_1. \tag{36}$$

Note that the terms in the square brackets are the unnormalized work moments; see Eq. (8), where $D(E)$ appears as the normalization of the probability of work.

In Fig. 4 we plot the unnormalized work moments to complement our numerical analysis. The upper panel shows $D\overline{W}_n/n!$ for a few odd n's, where the odd-moment-associated terms are all smooth functions of energy. Although decreasing in magnitudes with increasing n, $D\overline{W}_n/n!$ with higher n is not negligible, rather almost comparable, when compared to that of the lowest n. As combined with results of Fig. 3, it clearly means that the contributions of higher nth moments are negligible, not because their absolute magnitudes themselves or their first derivatives with respect to E are small, but because their n-order derivatives are diminishing with large n. Qualitatively, the same behavior is observed for those terms given by even number, n. These observations explain why the conjecture (36) works and, therefore, the almost perfect linear relation between the work average $\overline{W}_1$ and $\overline{W}_2$ displayed in Fig. 2(a).

Recently, the notion of stiffness was introduced as a sufficient condition for the Jarzynski equality to hold for work performed on a system initially prepared in a microcanonical initial state [26,27]. Here stiffness requires that the force protocol is characterized by a transition probability from the initial energy to any final energy independent of the initial energy. This discussion parallels what we found from our sum rule for the canonical initial state. However, this condition is apparently not satisfied for the microcanonical initial states. As we have shown explicitly through our numerical

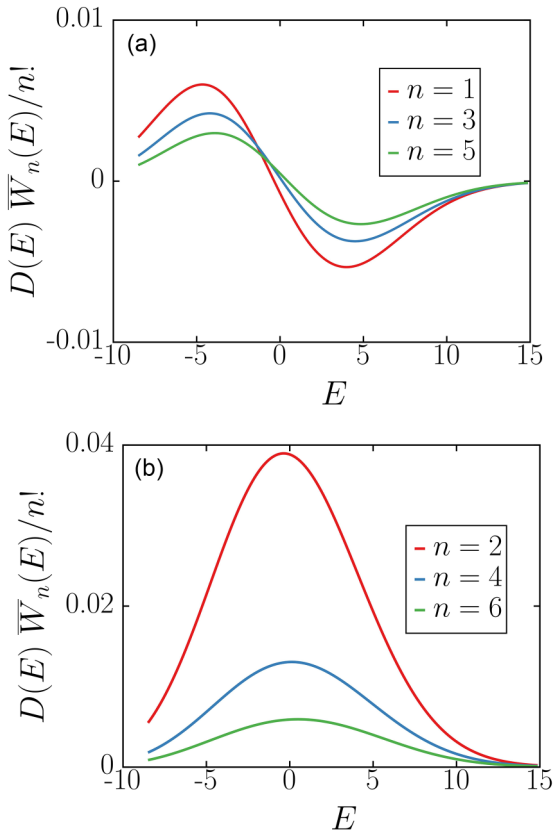

FIG. 4. Behaviors of the unnormalized work moments appearing in the sum rule (10) are displayed as a function of energy: (a) for odd n and (b) for even n.

calculations, even a weak perturbation yields work moments that depend on the initial energy, which directly proves that the stiffness condition is not fulfilled. On the other hand, our sum rule (10) states that the nth-order unnormalized work moment contributes to the work-fluctuation-governing law through not by itself but its nth derivatives with respect to the initial energy. Therefore, the nth-order contribution can be sufficiently small despite its energy dependence, leading to the approximate validity of the relation (24).

In closing, we point out the role of ϵ. We present the work average and the second moment of work for two different values of ϵ in Fig. 5. Recall here that disagreement between $M^{(2)}$ and the work average indicates the degree of the contributions from the higher-order work moments. In the case of a small decay scale (see the lower panel in which we choose ϵ to be 0.1 times the maximum level spacing) $M^{(2)}$ pronouncedly oscillates. This rapid oscillation discloses the discreteness of the energy spectra of the considered model system [28]. Most notably, $M^{(2)}$ deviates off the work average, meaning that the higher-order unnormalized work moments are susceptible to the energy location and make a non-negligible contribution to the sum rule. Only the relatively large decay scale (such as 1.5 times the maximum level spacing) tames such sensitivity and reduce their contribution to the sum rule, as displayed in Fig. 5(a).

In the seminal paper [12], the authors predicted that many repeated applications of cyclic perturbations of very short

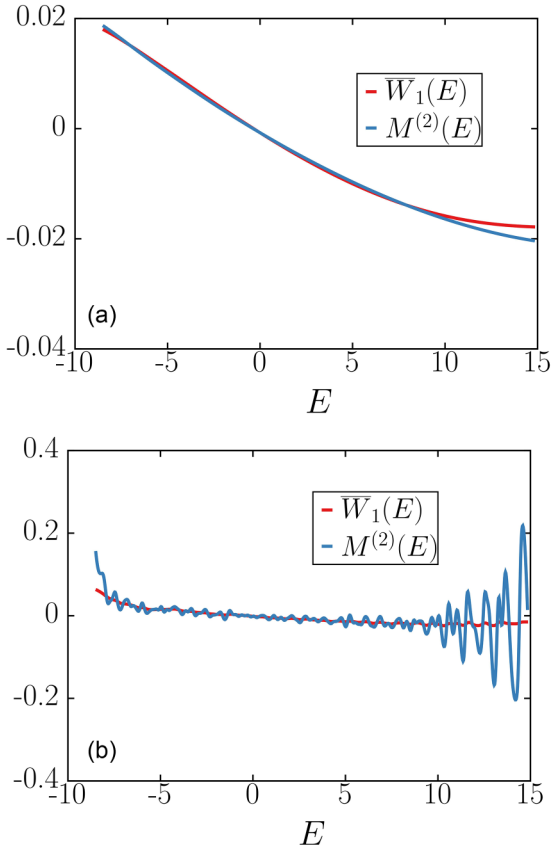

FIG. 5. $M^{(2)}(E)$ and work average as a function of E. Panels (a) and (b) show the results for ϵ being 1.5 and 0.1 times the maximum level spacing, respectively.

time intervals acting on an isolated quantum system lead to a universal non-Gibbssian ensemble. The basic equation of their theory is the Fokker-Planck equation of an energy distribution function. In Appendix B we show that the time evolution of the probability distribution function of energy can be written in terms of the work moments using the Kramers-Moyal (KM) expansion scheme and derive the Fokker-Planck (FP) equation by neglecting higher-order derivatives of work moments. The Fokker-Planck equation is adequate, at least when the higher-order work moments that appear in the KM expansion are not too sensitive to the energy location. Note that the work moments appearing in the KM expansion are the work moments in the limit $\epsilon \to 0$, and their time-average behaviors are very sensitive to E as observed in Fig. 5. When setting the perturbation interval very short, whether this E sensitivity diminishes so that the FP equation provides a valid description would require close investigation, from which we expect to understand an intriguing interplay between ϵ and the perturbation time interval.

V. SUMMARY

We have studied the fluctuating nature of work performed by a weak cyclic perturbation applied to a quantum system. We have derived an exact sum rule (10) governing the relation between work average and work fluctuation. Through the sum rule, we have shown that a linear relationship (24) between the first and the second moments of work can be obtained. Although it looks similar to previously postulated relation (1), our result (24) is different in that (i) it is not restricted to systems with Gaussian work distributions and (ii) the proportionality coefficient is defined via the derivatives not of the density of states $\omega(E)$ but of the normalization factor $D(E)$, so readily accessible even for a system with discrete energy spectrum. We also could identify that the essential element to allow the Jarzynski-type relation is the energy independence of the work moments in the case of the canonical initial states.

We have chosen a specific model system and a weak perturbation to numerically demonstrate the validity of the approximate relation (1). The perturbation we choose has a weak strength and short range, acting only on a small part of the system. Also, the force protocol taken here is a simple quench type. Such a choice of force protocol may be considered special. How not only model specifics, the range/strength of the acting perturbation, but also the time trajectory of perturbation alter the relation between work moments are not analysed in this study. We believe the subject is worthy of further research and anticipate that the derived sum rule (10) would guide understanding the specific behaviors of work fluctuations resulting from all those details.

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APPENDIX A: REDUCED DENSITY OPERATOR OF THE SMALL SUBSYSTEM OF A TOTAL SYSTEM DESCRIBED BY EQ. (2): CONNECTION TO THE CANONICAL ENSEMBLE

Let us suppose that a system described by $\hat{H}_0$ consists of a small subpart and the remainder (bath) weakly coupled to it. Neglecting the weak coupling, we can write the system Hamiltonian as $\hat{H}_0 = \hat{H}_s + \hat{H}_b$, in which $\hat{H}_s$ and $\hat{H}_b$ are the Hamiltonians of the small subpart and the bath, respectively. We let $\hat{H}_s|\Psi_j\rangle = \varepsilon_j|\Psi_j\rangle$, and $\hat{H}_b|\Gamma_k\rangle = B_k|\Gamma_k\rangle$. The eigenprojector of H_0 can be written as the linear combinations of the product state $|\Psi_j\rangle|\Gamma_k\rangle$:

$$\hat{\Pi}_i = \sum_{j,k} |\Psi_j\rangle\langle\Psi_j| \otimes |\Gamma_k\rangle\langle\Gamma_k| \delta_{E_i-\varepsilon_j-B_k} , \tag{A1}$$

which enters in Eq. (2). Note that only the pairs of (j,k) for which $\varepsilon_j + B_k = E_i$ is satisfied should contribute to the above sum. Upon the explicit inclusion of the weak coupling, the projector in general is not written in terms of such direct product state, and the issue becomes more involved in the proof of eigenstate thermalization hypothesis, which is elaboratively analyzed in Ref. [29].

The ensemble of the small subpart, $\hat{\rho}_s$, is determined by the partial trace over the bath as

$$\hat{\rho}_s = \mathrm{Tr}_b \hat{\rho}, \tag{A2}$$

which, upon using Eq. (2) and expressing the projector $\hat{\Pi}_i$ in terms of Eq. (A1), becomes

$$\hat{\rho}_s = \mathcal{N} \sum_j C_j |\Psi_j\rangle\langle\Psi_j|, \tag{A3}$$

where $\mathcal{N}$ is the normalization factor determined by $\mathrm{Tr}_s \hat{\rho}_s = 1$. Here the probability weight for the occupancy of the state $|\Psi_j\rangle$ (apart from the normalization factor) is given by

$$C_j = \sum_i m_i(E) \sum_k \delta_{B_k+\varepsilon_j-E_i} \tag{A4}$$

$$= \sum_k m\left(\frac{E-\varepsilon_j-B_k}{\epsilon}\right) \equiv D_b(E-\varepsilon_j). \tag{A5}$$

Therefore, the normalized reduced density operator for the small subsystem is determined as

$$\hat{\rho}_s = \frac{\sum_j D_b(E-\varepsilon_j)|\Psi_j\rangle\langle\Psi_j|}{\sum_j D_b(E-\varepsilon_j)}. \tag{A6}$$

When ϵ in function $m(x)$ [Eq. (4), for example] is comparable to the maximum level spacing of B_k's, $D_b(E-\varepsilon_j)$ is an almost continuous function of E. The continuity of $D_b(E)$ allows Taylor expansion, $D_b(E-\varepsilon_j) \sim \exp[-\beta(E)\varepsilon_j]$, under the assumption that ε_j is much smaller than E and $\beta(E) = \partial \ln D_b(E)/\partial E$ is constant, leading to the canonical ensemble.

APPENDIX B: KRAMERS-MOYAL EXPANSION

Consider in this Appendix a cyclic perturbation of a short time duration dt is repeatedly applied to an initial ensemble. The cyclic perturbation means that an instantaneous Hamiltonian at time t, $\hat{H}(t)$, is recovered at time $t+dt$; that is, $\hat{H}(t+dt) = \hat{H}(t)$. The time evolution of a density matrix $\hat{\rho}(t)$ that describes a system ensemble at time t is determined as

$$\hat{\rho}(t+dt) = U(t+dt,t)\hat{\rho}(t)U^\dagger(t+dt,t), \tag{B1}$$

where $U(t+dt,t)$ is the time evolution operator from time t to time $t+dt$. In general, $\hat{\rho}(t)$ is not diagonal in the eigenbasis of the Hamiltonian at an instant t. To acquire the energy distribution, we must introduce a crucial assumption: that $\hat{\rho}(t)$ is diagonal in the energy basis:

$$\hat{\rho}(t) = \sum_i \hat{\Pi}_i p_i(t). \tag{B2}$$

This assumption also applies to $\hat{\rho}(t+dt)$:

$$\hat{\rho}(t+dt) = \sum_i \hat{\Pi}_i p_i(t+dt). \tag{B3}$$

Inserting Eqs. (B3) and (B2) into Eq. (B1), we get

$$\mathrm{Tr}\hat{\Pi}_j(t)\hat{\rho}(t+dt) = d_{E_j} p_j(t+dt)$$
$$= \sum_i \mathrm{Tr}\hat{\Pi}_j U(t+dt,t) \times \hat{\Pi}_i U^\dagger(t+dt,t) p_i(t). \tag{B4}$$

and accordingly, an equation for the probability density function (PDF) of energy,

$$P(E,t+dt) \equiv \sum_j \delta(E-E_j) d_{E_j} p_j(t+dt)$$
$$= \sum_{ij} \delta(E-E_j)\mathrm{Tr}\hat{\Pi}_j U(t+dt,t) \times \hat{\Pi}_i U^\dagger(t+dt,t) p_i(t). \tag{B5}$$

Let us express the right-hand-side of (B5) in terms of the PDF at time t, given by

$$P(E,t) = \sum_i \delta(E-E_i) d_{E_i} p_i(t). \tag{B6}$$

In doing so, it is also necessary to introduce a probability of work,

$$P_W^I(E) = d_E^{-1} \sum_{ij} \left[\delta_{W-E_j+E_i}\left(\mathrm{Tr}\hat{\Pi}_j U(t+dt,t) \times \hat{\Pi}_i U^\dagger(t+dt,t)\right) I(E-E_i)\right], \tag{B7}$$

where $I(E-E_i)$ is an indicator function, which is unity if $E = E_i$ and zero otherwise. The normalization factor is given by $d_E = \sum_i \mathrm{Tr}\hat{\Pi}_i I(E-E_i)$. We add the superscript I in order to distinguish from the probability of work given in Eq. (8). $P_W^I(E)$ is related to $P_W(E)$ via

$$\lim_{\epsilon\to 0} P_W(E) = P_W^I(E), \tag{B8}$$

where the limit applies to $m_i(E)$ built in $P_W(E)$ as

$$\lim_{\epsilon\to 0} m_i(E) = \lim_{\epsilon\to 0} \frac{2}{1+\cosh[(E-E_i)/\epsilon]} \approx I(E-E_i) = \begin{cases} 1 & \text{if } E = E_i \\ 0 & \text{otherwise.} \end{cases}$$

By inspection, we find

$$P(E,t+dt) = \sum_W P_W^I(E-W) P(E-W,t). \tag{B9}$$

The validity of this relation can be checked by inserting Eqs. (B6) and (B7) into (B9) and comparing the outcome with Eq. (B5). Equation (B9) is also identical to what is given in Ref. [30]; see Sec. 6.4 therein.

We expand $P_W(E-W)$ and $P(E-W,t)$ as a power series of W in their function arguments:

$$P_W^I(E-W) = \sum_{\ell=0}^{\infty} (-1)^\ell (W^\ell/\ell!)\partial_E^\ell P_W^I(E), \tag{B10}$$

$$P(E-W,t) = \sum_{m=0}^{\infty} (-1)^m (W^m/m!)\partial_E^m P(E,t) \tag{B11}$$

with $\partial_E^\ell = (\partial/\partial E)^\ell$. Inserting these expansions into Eq. (B9), and defining the nth moment of work as

$$W_n^I(E) = \sum_W W^n P_W^I(E), \tag{B12}$$

we get

$$P(E,t+dt) = \sum_{\ell,m}(-1)^{\ell+m}\left[\partial_E^{\ell} W^I_{\ell+n}(E)\right]\partial_E^m P(E,t)$$
$$= \sum_{n=0}^{\infty}\frac{(-1)^n}{n!}\partial_E^n\left\{W_n^I(E)P(E,t)\right\}, \qquad \text{(B13)}$$

where the use the Leibniz rule acquires the second equality. This equation is akin to the Kramers-Moyal expansion connecting the energy distribution function at time $t+dt$ and that at time t through the moment of work.

Writing a few terms in Eq. (B13) explicitly as

$$P(E,t+dt) - P(E,t)$$
$$= -\partial_E[W_1^I P(E,t)] + \tfrac{1}{2}\partial_E^2[W_2^I P(E,t)] + \cdots, \qquad \text{(B14)}$$

we find that the above equation becomes the Fokker-Planck equation with drift W_1^I/dt and diffusion constant W_2^I/dt in the energy space when the higher order derivatives $\partial_E^{n\geqslant 3}$ of $W_n^I P(E,t)$ are negligible.

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