Tensor-network approach to work statistics for one-dimensional quantum lattice systems

Jiayin Gu [1,*] Fan Zhang,[1] and H. T. Quan [1,2,3,†]
[1]*School of Physics, Peking University, Beijing 100871, China*
[2]*Collaborative Innovation Center of Quantum Matter, Beijing 100871, China*
[3]*Frontiers Science Center for Nano-Optoelectronics, Peking University, Beijing 100871, China*

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We introduce a tensor-network approach to calculate the statistics of work done on one-dimensional quantum lattice systems initially prepared in thermal equilibrium states. In this approach, the dynamics is simulated with time-evolving block decimation (TEBD), and the initial thermal equilibrium state is prepared either directly with TEBD or with minimally entangled typical thermal states, which generates a set of typical states representing the Gibbs canonical ensemble. As an illustrative example, we apply this approach to the Ising chain in mixed transverse and longitudinal fields. Under a prescribed protocol, the moment generating function for work distribution can be calculated, from which the quantum Jarzynski equality and the generalized quantum work relation involving a functional of an arbitrary observable are tested.

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I. INTRODUCTION

Microreversibility, a fundamental symmetry of nature, dictates various nonequilibrium relations, which are nowadays collectively known as fluctuation theorems [1–9]. Among these relations, the Jarzynski equality attracts considerable interests. It is a parameter-free, model-independent relation, and allows us to express the free-energy difference between two equilibrium states by a nonlinear average over the required work to drive the system in a nonequilibrium process from one state to another. Over the last decades, extensive efforts were devoted to proving and experimentally testing the Jarzynski equality or its closely related Crooks fluctuation theorem in various systems [10–27]. However, what is more informative is the detailed probability distribution of work under an arbitrary protocol (instead of a sudden quench [28,29]), since it encodes essential information about not only the equilibrium properties but also the nonequilibrium driving processes [19,20,30–38].

For quantum many-body systems, the reality is that it is formidably challenging to calculate the work statistics under an arbitrary driving protocol. Previous studies mainly focus on analytical methods and are restricted to few exactly solvable models which are studied case by case. Examples include harmonic oscillators [39–44], piston systems [45–47], one-dimensional (1D) diatomic Toda lattice [48], 1D quantum gases [47,49–51], quantum fields [52,53], and quantum systems of quadratic Hamiltonians [54–58]. The quantum Feynman-Kac equation [59] and the phase-space formulation [60–62] have been proposed, but they are practically limited to single-particle systems and difficult to extend to many-body systems. Nonequilibrium Green's function approach [63], group-theoretical approach [55,56], and path-integral approach [39,45,64–66] have been proposed, but they are only applicable to perturbative driving protocols and/or systems with quadratic Hamiltonians. Despite these efforts, a systematic method for calculating the work distribution of a quantum many-body system under an arbitrary driving protocol is still lacking. Thus, developing numerical ones becomes a natural consideration. The tensor-network approach [67,68] is an ideal candidate and drastically decreases the computation complexity associated with the exponentially large Hilbert space intrinsic to quantum many-body systems. Although originally developed in the context of condensed-matter physics, the tensor-network approach is increasingly being applied to tackle problems in other fields of research. In quantum thermodynamics, for example, the tensor-network approach has recently been used to simulate strongly interacting quantum thermal machines [69] and to study the heat transfer in non-Markovian open quantum systems [70].

In this Letter, we introduce a numerical approach to calculate the work statistics for 1D quantum lattice systems in nonequilibrium processes. Two tensor-network techniques are used, namely, time-evolving block decimation (TEBD) [71] and minimally entangled typical thermal states (METTS) [72]. The quantum Ising chain in the presence of transverse and longitudinal fields is chosen to benchmark this approach.

II. TWO-POINT MEASUREMENT SCHEME

In the nanoscopic world, the extension of classical Jarzynski equality to quantum systems can be realized through a proper definition of work introduced in the year 2000 [10,11].

*gujiayin@pku.edu.cn
†htquan@pku.edu.cn

In this scheme, a measurement of energy is initially performed on the system in a thermal equilibrium state. In the sequel, the system evolves under an external driving protocol before another measurement of energy at the final time τ. The fluctuating work is defined as the energy difference between the two eigenenergies, $W_{m,n} = E_m^\tau - E_n^0$. The joint probability of observing such measurement outcome is given by $\mathcal{P}(n,m) = \mathcal{P}_n |\langle m(\tau)|U|n(0)\rangle|^2$, where $|n(t)\rangle$ is the nth instantaneous energy eigenstate of the system at time t, $\mathcal{P}_n = \langle n(0)|\rho|n(0)\rangle$ the initial probability of $|n(0)\rangle$, $\rho = e^{-\beta H(0)}/Z$ the initial canonical density matrix of the system at the inverse temperature $\beta \equiv 1/(k_B T)$, and k_B the Boltzmann's constant. Besides, U denotes the unitary evolution operator, which is expressed in terms of the time-dependent Hamiltonian $H(t)$ and the time-ordering operator $\mathcal{T}$,

$$U = \mathcal{T} \exp\left[-\frac{i}{\hbar}\int_0^\tau H(t)dt\right]. \tag{1}$$

The work distribution is therefore given by $\mathcal{P}(W) = \sum_{m,n} \delta(W - W_{m,n})\mathcal{P}(m,n)$. We define the moment-generating function of the work distribution,

$$G(s) = \int \mathcal{P}(W) e^{sW} dW, \tag{2}$$

then the moment generating function can be expressed as

$$G(s) = \mathrm{Tr}[U^\dagger e^{sH(\tau)} U e^{-sH(0)} \rho]. \tag{3}$$

The moments of work can be obtained by taking successive derivatives,

$$\langle W^n \rangle = \left.\frac{d^n G(s)}{ds^n}\right|_{s=0}. \tag{4}$$

The moment-generating function (3) is the quantity that we will numerically calculate with the tensor-network approach.

III. TIME-EVOLVING BLOCK DECIMATION

TEBD is an algorithm that relies on the Trotter-Suzuki decomposition [73] and subsequent approximation of the exact evolution operator $U^{\mathrm{exact}}(\delta)$ for the small quantity δ. The full Hamiltonian H can be split into N_H parts, $H = \sum_{\alpha=1}^{N_H} H_\alpha$, where each part H_α is a sum, $H_\alpha = \sum_{k=1}^{N_\alpha} h_\alpha^k$, such that h_α^k can be diagonalized efficiently and are mutually commuting, $[h_\alpha^k, h_\alpha^l] = 0$. The exact evolution operator can be decomposed to any order. Here, we give the second-order one,

$$\begin{aligned} U^{\mathrm{exact}}(\delta) &= e^{-\delta \sum_{\alpha=1}^{N_H} H_\alpha} \\ &\approx \prod_{\alpha=1}^{N_H} e^{-\frac{\delta}{2} H_\alpha} \prod_{\alpha=N_H}^{1} e^{-\frac{\delta}{2} H_\alpha} + O(\delta^3), \end{aligned} \tag{5}$$

as it is commonly used. Figure 1 depicts the TEBD algorithm with diagrammatic notations.

IV. MINIMALLY ENTANGLED TYPICAL THERMAL STATES

METTS is a finite-temperature algorithm for generating a set of typical states representing the Gibbs canonical ensemble. For a quantum lattice system, starting from a product state

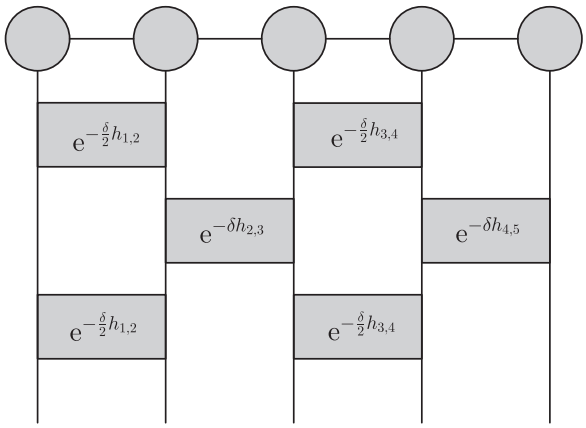

FIG. 1. Diagrammatic representation of the TEBD algorithm for a quantum lattice system of five sites with nearest-neighbor interactions. The full Hamiltonian is split into two parts, $H = H_{\mathrm{odd}} + H_{\mathrm{even}}$ with $H_{\mathrm{odd}} = h_{1,2} + h_{3,4}$ and $H_{\mathrm{even}} = h_{2,3} + h_{4,5}$. The odd and even numbered two-site local evolution operators are alternatively applied to the wave function represented by a matrix product state (MPS) [74].

$|i\rangle$, we can generate a typical state called metts $|\psi(i)\rangle$ with the imaginary time evolution,

$$|\psi(i)\rangle = \frac{1}{\sqrt{\mathcal{P}(i)}} e^{-\beta H/2} |i\rangle, \tag{6}$$

where $\mathcal{P}(i) = \langle i|e^{-\beta H}|i\rangle$. Here, the evolution is realized using TEBD. A set of metts satisfy the typicality condition,

$$\rho = \frac{e^{-\beta H}}{Z} = \sum_i \frac{\mathcal{P}(i)}{Z} |\psi(i)\rangle \langle\psi(i)|, \tag{7}$$

where Z denotes the partition function, and $\mathcal{P}(i)/Z$ is therefore the weight of $|\psi(i)\rangle$. The expectation value of an arbitrary static observable O can be calculated as

$$\langle O\rangle = \frac{1}{Z}\sum_i \mathcal{P}(i) \langle\psi(i)|O|\psi(i)\rangle, \tag{8}$$

To sample the metts ensemble randomly according to the probability distribution $\mathcal{P}(i)/Z$, we construct a Markov chain of the product state by first obtaining a metts $|\psi(i)\rangle$ from a product state $|i\rangle$, second collapsing the metts $|\psi(i)\rangle$ into a new product state $|j\rangle$ with the probability $\mathcal{P}(i \to j) = |\langle j|\psi(i)\rangle|^2$, and third repeating this procedure. $|i\rangle$ is henceforth referred to as a collapsed product state (cps). Considering the ensemble of all cps $|i\rangle$ initially distributed with probability $\mathcal{P}(i)/Z$, it can be checked that the detailed balance condition is satisfied,

$$\frac{\mathcal{P}(i)}{Z}\mathcal{P}(i \to j) = \frac{\mathcal{P}(j)}{Z}\mathcal{P}(j \to i), \tag{9}$$

guaranteeing the stability of the Markov chain. See Fig. 2 for a brief illustration of the METTS algorithm. Detailed accounts can be found in Ref. [75].

V. ILLUSTRATIVE EXAMPLE

We now consider a spin one-half quantum Ising chain of L sites with nearest-neighbor interactions in the presence of

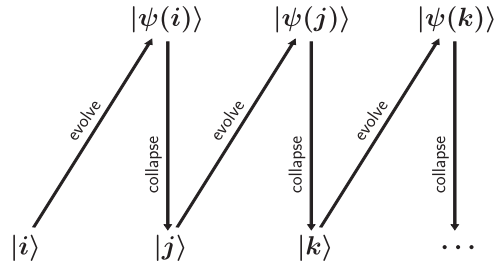

FIG. 2. Schematic representation of the METTS algorithm whose procedure consists of the following steps: (i) choose a cps $|i\rangle$; (ii) evolve it to a metts $|\psi(i)\rangle$ in imaginary time according to Eq. (6) and calculate quantities of interest; (iii) collapse $|\psi(i)\rangle$ into a new cps $|j\rangle$ with the probability $\mathcal{P}(i \to j) = |\langle j|\psi(i)\rangle|^2$ and then return to (ii).

transverse and longitudinal fields. The Hamiltonian is given by

$$H = -J \sum_{\langle j,j+1\rangle} S_j^z S_{j+1}^z - h_x \sum_j S_j^x - h_z \sum_j S_j^z, \tag{10}$$

where S_j^z and S_j^x denote the spin operators at the jth site defined in terms of Pauli matrices,

$$S_j^x = \frac{\sigma^x}{2} = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad S_j^z = \frac{\sigma^z}{2} = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \tag{11}$$

and J is the exchange constant. h_x (h_z) is the magnetic field in x (z) direction controlled externally in time according to a prescribed protocol, thus making the Hamiltonian time dependent. Different from the transverse-field Ising chain, the Ising chain in mixed fields cannot be solved exactly. We have to resort to a numerical approach for a detailed investigation.

To fit into the TEBD algorithm, the full Hamiltonian is split into odd and even parts, $H = H_{\text{odd}} + H_{\text{even}}$, with H_{odd} and H_{even} each being the sum of mutually commuting local two-site operators,

$$H_{\text{odd}} = \sum_{j\in\text{oddset}} h_{j,j+1}, H_{\text{even}} = \sum_{j\in\text{evenset}} h_{j,j+1}, \tag{12}$$

as illustrated in Fig. 1. Each local two-site operator $h_{j,j+1}$ is constructed as follows:

$$\begin{aligned} h_{j,j+1} = &- JS_j^z \otimes S_{j+1}^z \\ &- \frac{(1+\delta_{j,1})\left(h_x S_j^x \otimes \mathsf{I}_{j+1}\right)}{2} \\ &- \frac{(1+\delta_{j+1,L})\left(\mathsf{I}_j \otimes h_x S_{j+1}^x\right)}{2} \\ &- \frac{(1+\delta_{j,1})\left(h_z S_j^z \otimes \mathsf{I}_{j+1}\right)}{2} \\ &- \frac{(1+\delta_{j+1,L})\left(\mathsf{I}_j \otimes h_z S_{j+1}^z\right)}{2}, \end{aligned} \tag{13}$$

where $\otimes$ stands for the tensor product, $\delta_{i,j}$ is the Kronecker delta, and I_j is the identity operator at the jth site.

Using the METTS algorithm, we can successively generate a set of metts $\{|\psi_\alpha\rangle\}_{\alpha=1}^N$ for the Hamiltonian $H(0)$ at the initial time. Considering that the occurrence frequency of

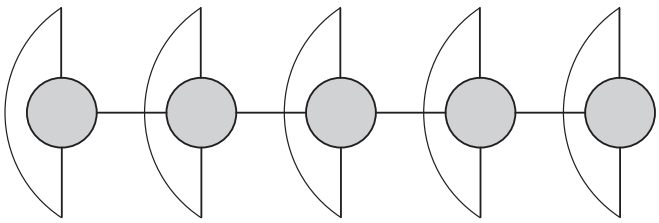

FIG. 3. The partition function is calculated by tracing out two sets of physical indices of the MPO representing $\exp(-\beta H)$.

$|\psi_\alpha\rangle \equiv |\psi(i)\rangle$ is asymptotically equal to $\mathcal{P}(i)/Z$ as $N \to \infty$, the initial canonical density matrix (7) can be expressed as

$$\rho = \lim_{N\to\infty} \frac{1}{N} \sum_{\alpha=1}^{N} |\psi_\alpha\rangle \langle\psi_\alpha| . \tag{14}$$

The moment generating function (3) is therefore given by

$$\begin{aligned} G(s) &= \lim_{N\to\infty} \frac{1}{N} \sum_{\alpha=1}^{N} \text{Tr}[|\phi_\alpha\rangle \langle\psi_\alpha|] \\ &= \lim_{N\to\infty} \frac{1}{N} \sum_{\alpha=1}^{N} \langle\psi_\alpha|\phi_\alpha\rangle , \end{aligned} \tag{15}$$

where

$$|\phi_\alpha\rangle = U^\dagger e^{sH(\tau)} U e^{-sH(0)} |\psi_\alpha\rangle \tag{16}$$

is calculated with the TEBD algorithm. It is noteworthy that this approach is also capable of calculating the work statistics if the system evolves starting from the ground state. Usually, the density matrix renormalization group (DMRG) [76,77] is used to find the ground state of quantum many-body systems. In our approach, however, the ground state can be obtained with imaginary time evolution in the low-temperature limit, i.e., calculated from Eq. (6) in the limit $\beta \to \infty$, only if the initial cps $|i\rangle$ has the component of the ground state.[1] It converges exponentially fast and is also computationally efficient since the ground state is well represented as a MPS. In addition, there is no need to generate an ensemble of states, in contrast with the finite-temperature case.

According to the definition of moment generating function (2), we have $\langle\exp(-\beta W)\rangle \equiv G(-\beta)$. To check whether the numerical approach gives the correct work statistics satisfying the Jarzynski equality, the quantity $\exp(-\beta\Delta F) \equiv Z(h_{x,\tau}, h_{z,\tau})/Z(h_{x,0}, h_{z,0})$ should be calculated differently. This can be done through the definition of the partition function, $Z \equiv \text{Tr}[\exp(-\beta H)]$, where $\exp(-\beta H)$ is expressed as a matrix product operator (MPO). We first prepare an initial identity MPO, $\delta_{j_1,j_1'}\delta_{j_2,j_2'}\cdots\delta_{j_L,j_L'}$, and then evolve it under $\exp(-\beta H)$ with the TEBD algorithm to obtain the desired MPO. The tracing operation is now transformed into tensor contraction (see a diagrammatic illustration in Fig. 3).

Now, we perform numerical simulation. We calculate both $G(-\beta)$ and $Z(h_{x,\tau}, h_{z,\tau})/Z(h_{x,0}, h_{z,0})$ for various driving time

[1]Due to the round-off error in numerical computation, the component of ground state is inevitably introduced during imaginary time evolution.

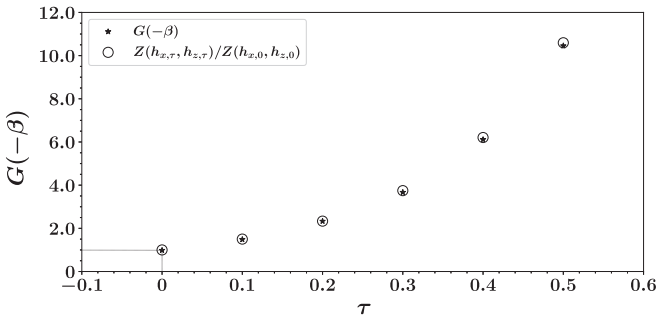

FIG. 4. Moment-generating function $G(-\beta)$ calculated for different time intervals $[0, \tau]$ during which the system is driven under the protocol $h_x(t) = t + 1$, $h_z = 1$. The corresponding values of $Z(h_{x,\tau}, h_{z,\tau})/Z(h_{x,0}, h_{z,0})$ are also marked. When there is no driving, i.e., $\tau = 0$, we have $G(-\beta) = 1$, as it should be. The system is composed of $L = 20$ sites and the parameter values $J = \beta = \hbar = 1$ are adopted. 10 000 metts are generated in the simulation.

intervals $[0, \tau]$ and compare their values. The results are shown in Fig. 4, from which we see a striking agreement. Therefore, the quantum Jarzynski equality, $\langle \exp(-\beta W) \rangle = \exp(-\beta \Delta F)$, is tested. Here, we would like to emphasize that the canonical density matrix is represented by a set of metts for the left-hand side, and constructed directly for the right-hand side. If the density matrices for both sides were constructed in the same way, the comparison would be meaningless since the quantum Jarzynski equality is actually an identity.

A generalized quantum work relation was proved in Ref. [78]. It reads

$$\left\langle e^{\int_0^\tau \lambda(t) O_{\rm F}^{\rm H}(t) dt} e^{-\beta H_{\rm F}^{\rm H}(\tau)} e^{\beta H(0)} \right\rangle_{\rm F} = e^{-\beta \Delta F} \left\langle e^{\int_0^\tau \lambda(\tau - t) O_{\rm R}^{\rm H}(t) dt} \right\rangle_{\rm R}, \tag{17}$$

which involves an arbitrary function $\lambda(t)$ and an arbitrary time-independent observable O. In this relation, $H_{\rm F}^{\rm H}(t) \equiv U_{\rm F}^\dagger(t) H(t) U_{\rm F}(t)$, $O_{\rm F}^{\rm H}(t) \equiv U_{\rm F}^\dagger(t) O U_{\rm F}(t)$ are respectively the Hamiltonian and the observable in the Heisenberg picture for the forward process. $O_{\rm R}^{\rm H}(t) \equiv U_{\rm R}^\dagger(t) O U_{\rm R}(t)$ is the observable in the Heisenberg picture for the reversed process. The unitary evolution operators for both processes are given by $U_{\rm F}(t) = \mathcal{T} \exp[\int_0^t H(t')/(i\hbar) dt']$ and $U_{\rm R}(t) = \mathcal{T} \exp[\int_0^t H(\tau - t')/(i\hbar) dt']$. The symbols $\langle \cdot \rangle_{\rm F}$ and $\langle \cdot \rangle_{\rm R}$ denote the average over the initial canonical ensemble for the forward and the reversed processes, i.e., the density matrices determined by the Hamiltonian $H(0)$ and $H(\tau)$, respectively. It should be noted here that we have neglected the issue relevant to time reversal, for the sake of convenience in the subsequent numerical simulation. In other words, all observables are supposed to be even under time reversal, $\Theta O \Theta = O$. When $\lambda(t) = 0$, the relation (17) reduces to the familiar quantum Jarzynski equality, $\langle e^{-\beta H_{\rm F}^{\rm H}(\tau)} e^{\beta H(0)} \rangle_{\rm F} = e^{-\beta \Delta F}$, where, in the two-point measurement scheme, the factor inside the bracket can be interpreted in terms of work performed on the system during the forward process. With the Ising chain considered previously, we now numerically test the relation (17). The observable is chosen to be the magnetization along the z direction, $O = \sum_j S_j^z$, which can be split into odd and even parts in a similar manner to the case of the Hamiltonian. The initial canonical ensemble for the forward and the reversed processes are generated with METTS. The operators inside the brackets of Eq. (17) are calculated with TEBD. The numerical results are presented in Table I with three cases of the function $\lambda(t)$. The last column lists the ratio between two sides of Eq. (17). The values are approximately equal to 1, in good agreement with the theory.

TABLE I. The numerical results testing the Eq. (17) with three cases of $\lambda(t)$. A represents the left-hand side, B, C, respectively, $e^{-\beta \Delta F}$ and the other part of the right-hand side. The system is composed of $L = 20$ sites, and is driven in time under the protocol $h_x(t) = t + 1$ [$h_x(t) = 1.5 - t$], $h_z = 1$ from 0 to $\tau = 0.5$ for the forward (reversed) process. The parameter values $J = \beta = \hbar = 1$ are adopted. 5000 metts are generated for each ensemble.

	A	B	C	BC/A
$\lambda(t) = 1$	254.316	10.596	23.371	0.974
$\lambda(t) = t + 1$	641.533	10.596	61.366	1.014
$\lambda(t) = t^2 + t + 1$	907.979	10.596	85.142	0.994

The successful tests of the quantum Jarzynski equality and its generalized version manifest the reliability of our tensor-network approach. We now calculate $G(s)$ for a specific protocol (see Fig. 5). To reduce the cost of computational resources, the initial canonical density matrix is here constructed directly. In this way, we can perform simulation for systems with a large number of lattice sites in a reasonable time. We here calculate $G(s)$ for the system with 100 lattice sites. This system size is far beyond the capability of computation with exact matrix representation. According to Eq. (4), the work moments are evaluated with numerical differentiation which can be achieved through Lagrange interpolation [79]. In this way, we can reliably obtain the expected value and its variance without sampling. A relevant approach for estimating the expected value based on tensor networks was reported in Ref. [80].

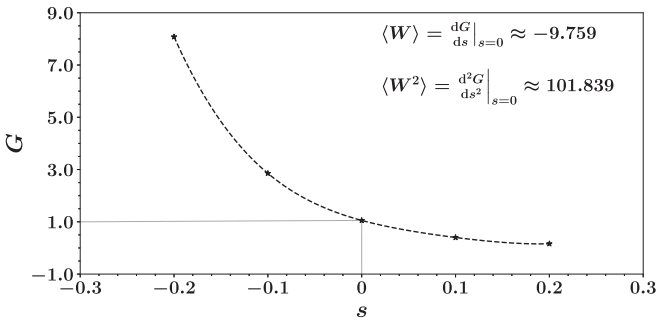

FIG. 5. Moment-generating function $G(s)$. The asterisks are numerical points joined by a dashed line determined from Lagrange interpolation. It has been checked that to a very high precision $G(0) \approx 1$, as expected. The first and the second work moments are evaluated with numerical differentiation. The system is composed of $L = 100$ sites, and is driven in time from $t = 0$ to $t = 0.5$ under the protocol $h_x(t) = t + 1$, $h_z = 1$. The parameter values $J = \beta = \hbar = 1$ are adopted. The initial canonical density matrix is constructed directly.

The computer program for numerical simulation is coded in C++ [81] with the ITensor library [82]. A comprehensive and up-to-date snapshot of software for tensor computations is assembled in Ref. [83].

VI. CONCLUSION

In this Letter, we introduced a tensor-network approach for calculating the work statistics of 1D quantum lattice systems. This numerical approach enables the detailed investigation of the work statistics under an arbitrary nonperturbative protocol. Therefore, our numerical approach is expected to find further applications in the design of quantum devices operating in nonequilibrium regimes. Besides the work statistics, we can also calculate many other dynamical quantities with this method, such as Loschmidt echo, information scrambling, and density of topological defects associated with Kibble-Zurek scaling. Extension of the numerical approach to high-dimensional systems will be considered in the future.

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[1] G. N. Bochkov and Y. E. Kuzovlev, General theory of thermal fluctuations in nonlinear systems, Sov. J. Exp. Theor. Phys. **45**, 125 (1977).
[2] D. J. Evans, E. G. D. Cohen, and G. P. Morriss, Probability of Second Law Violations in Shearing Steady States, Phys. Rev. Lett. **71**, 2401 (1993).
[3] G. Gallavotti and E. G. D. Cohen, Dynamical Ensembles in Nonequilibrium Statistical Mechanics, Phys. Rev. Lett. **74**, 2694 (1995).
[4] C. Jarzynski, Nonequilibrium Equality for Free Energy Differences, Phys. Rev. Lett. **78**, 2690 (1997).
[5] J. Kurchan, Fluctuation theorem for stochastic dynamics, J. Phys. A: Math. Gen. **31**, 3719 (1998).
[6] G. E. Crooks, Entropy production fluctuation theorem and the nonequilibrium work relation for free energy differences, Phys. Rev. E **60**, 2721 (1999).
[7] J. L. Lebowitz and H. Spohn, A Gallavotti-Cohen-type symmetry in the large deviation functional for stochastic dynamics, J. Stat. Phys. **95**, 333 (1999).
[8] C. Maes, The fluctuation theorem as a Gibbs property, J. Stat. Phys. **95**, 367 (1999).
[9] U. Seifert, Stochastic thermodynamics: Principles and perspectives, Eur. Phys. J. B **64**, 423 (2008).
[10] H. Tasaki, Jarzynski relations for quantum systems and some applications, arXiv:cond-mat/0009244.
[11] J. Kurchan, A quantum fluctuation theorem, arXiv:cond-mat/0007360.
[12] W. De Roeck and C. Maes, Quantum version of free-energy-irreversible-work relations, Phys. Rev. E **69**, 026115 (2004).
[13] P. Talkner, E. Lutz, and P. Hänggi, Fluctuation theorem: Work is not an observable, Phys. Rev. E **75**, 050102(R) (2007).
[14] G. Huber, F. Schmidt-Kaler, S. Deffner, and E. Lutz, Employing Trapped Cold Ions to Verify the Quantum Jarzynski Equality, Phys. Rev. Lett. **101**, 070403 (2008).
[15] C. Jarzynskia, Nonequilibrium work relations: Foundations and applications, Eur. Phys. J. B **64**, 331 (2008).
[16] C. Jarzynski, Equalities and inequilities: Irreversibility and the second law of thermodynamics at the nanoscale, Annu. Rev. Condens. Matter Phys. **2**, 329 (2011).
[17] M. Esposito, U. Harbola, and S. Mukamel, Nonequilibrium fluctuations, fluctuation theorems, and counting statistics in quantum systems, Rev. Mod. Phys. **81**, 1665 (2009).
[18] M. Campisi, P. Hänggi, and P. Talkner, Colloquium: Quantum fluctuation relations: Foundations and applications, Rev. Mod. Phys. **83**, 771 (2011).
[19] R. Dorner, S. R. Clark, L. Heaney, R. Fazio, J. Goold, and V. Vedral, Extracting Quantum Work Statistics and Fluctuation Theorems by Single-Qubit Interferometry, Phys. Rev. Lett. **110**, 230601 (2013).
[20] L. Mazzola, G. D. Chiara, and M. Paternostro, Measuring the Characteristic Function of the Work Distribution, Phys. Rev. Lett. **110**, 230602 (2013).
[21] R. Klages, W. Just, and C. Jarzynski, eds., *Nonequilibrium Statistical Physics of Small Systems: Fluctuation Relations and Beyond* (Wiley-VCH, 2013).
[22] T. B. Batalhão, A. M. Souza, L. Mazzola, R. Auccaise, R. S. Sarthour, I. S. Oliveira, J. Goold, G. D. Chiara, M. Paternostro, and R. M. Serra, Experimental Reconstruction of Work Distribution and Study of Fluctuation Relations in a Closed Quantum System, Phys. Rev. Lett. **113**, 140601 (2014).
[23] G. Hummer and A. Szabo, Free energy profile from single-molecule pulling experiments, Proc. Natl. Acad. Sci. USA **107**, 21441 (2010).
[24] J. Liphardt, S. Dumont, S. B. Smith, I. Tinoco Jr., and C. Bustamante, Equilibrium information from nonequilibrium measurements in an experimental test of Jarzynski's equality, Science **296**, 1832 (2002).
[25] D. Collin, F. Ritort, C. Jarzynski, S. B. Smith, I. T. Jr, and C. Bustamante, Verification of the crooks fluctuation theorem and recovery of RNA folding free energies, Nature (London) **437**, 231 (2005).
[26] S. An, J.-N. Zhang, M. Um, D. Lv, Y. Lu, J. Zhang, Z.-Q. Yin, H. T. Quan, and K. Kim, Experimental test of the quantum Jarzynski equality with a trapped-ion system, Nat. Phys. **11**, 193 (2015).
[27] T. M. Hoang, R. Pan, J. Ahn, J. Bang, H. T. Quan, and T. Li, Experimental Test of the Differential Fluctuation Theorem and a Generalized Jarzynski Equality for Arbitrary Initial States, Phys. Rev. Lett. **120**, 080602 (2018).

[28] E. G. Arrais, D. A. Wisniacki, L. C. Céleri, N. G. de Almeida, A. J. Roncaglia, and F. Toscano, Quantum work for sudden quenches in Gaussian random Hamiltonians, Phys. Rev. E **98**, 012106 (2018).

[29] E. G. Arrais, D. A. Wisniacki, A. J. Roncaglia, and F. Toscano, Work statistics for sudden quenches in interacting quantum many-body systems, Phys. Rev. E **100**, 052136 (2019).

[30] M. Heyl, A. Polkovnikov, and S. Kehrein, Dynamical Quantum Phase Transitions in the Transverse-Field Ising Model, Phys. Rev. Lett. **110**, 135704 (2013).

[31] A. Silva, Statistics of the Work Done on a Quantum Critical System by Quenching a Control Parameter, Phys. Rev. Lett. **101**, 120603 (2008).

[32] B. Dóra, Ádám Bácsi, and G. Zaránd, Generalized Gibbs ensemble and work statistics of a quenched Luttinger liquid, Phys. Rev. B **86**, 161109(R) (2012).

[33] A. Russomanno, S. Sharma, A. Dutta, and G. E. Santoro, Asymptotic work statistics of periodically driven Ising chains, J. Stat. Mech.: Theory Exp. (2015), P08030.

[34] C. Jarzynski, H. T. Quan, and S. Rahav, Quantum-Classical Correspondence Principle for Work Distributions, Phys. Rev. X **5**, 031038 (2015).

[35] L. Zhu, Z. Gong, B. Wu, and H. T. Quan, Quantum-classical correspondence principle for work distributions in a chaotic system, Phys. Rev. E **93**, 062108 (2016).

[36] Q. Wang and H. T. Quan, Understanding quantum work in a quantum many-body system, Phys. Rev. E **95**, 032113 (2017).

[37] J. Goold, F. Plastina, A. Gambassi, and A. Silva, The role of quantum work statistics in many-body physics, in *Thermodynamics in the Quantum Regime: Fundamental Aspects and New Directions* (Springer, 2018).

[38] K. Beyer, K. Luoma, and W. T. Strunz, Work as an external quantum observable and an operational quantum work fluctuation theorem, Phys. Rev. Research **2**, 033508 (2020).

[39] K. Funo and H. T. Quan, Path Integral Approach to Quantum Thermodynamics, Phys. Rev. Lett. **121**, 040602 (2018).

[40] S. Deffner and E. Lutz, Nonequilibrium work distribution of a quantum harmonic oscillator, Phys. Rev. E **77**, 021128 (2008).

[41] P. Talkner, P. Sekhar, and P. Hänggi, Statistics of work performed on a forced quantum oscillator, Phys. Rev. E **78**, 011115 (2008).

[42] J. D. Jaramillo, J. Deng, and J. Gong, Quantum work fluctuations in connection with the Jarzynski equality, Phys. Rev. E **96**, 042119 (2017).

[43] H. K. Yadalam and U. Harbola, Statistics of work done in a degenerate parametric amplification process, Phys. Rev. A **99**, 063802 (2019).

[44] N. M. Myers and S. Deffner, Bosons outperform fermions: The thermodynamic advantage of symmetry, Phys. Rev. E **101**, 012110 (2020).

[45] T. Qiu, Z. Fei, R. Pan, and H. T. Quan, Path-integral approach to the calculation of the characteristic function of work, Phys. Rev. E **101**, 032111 (2020).

[46] H. T. Quan and C. Jarzynsk, Validity of nonequilibrium work relations for the rapidly expanding quantum piston, Phys. Rev. E **85**, 031102 (2012).

[47] Z. Gong, S. Deffner, and H. T. Quan, Interference of identical particles and the quantum work distribution, Phys. Rev. E **90**, 062121 (2014).

[48] L. Zhu and J. Wang, Calculating the free energy difference by applying the jarzynski equality to a virtual integrable system, Phys. Rev. E **98**, 022117 (2018).

[49] Y. Zheng and D. Poletti, Quantum statistics and the performance of engine cycles, Phys. Rev. E **92**, 012110 (2015).

[50] B. Wang, J. Zhang, and H. T. Quan, Work distributions of one-dimensional fermions and bosons with dual contact interactions, Phys. Rev. E **97**, 052136 (2018).

[51] Y. Y. Atas, A. Safavi-Naini, and K. V. Kheruntsyan, Nonequilibrium quantum thermodynamics of determinantal many-body systems: Application to the Tonks-Girardeau and ideal Fermi gases, Phys. Rev. A **102**, 043312 (2020).

[52] A. Ortega, E. McKay, Álvaro M. Alhambra, and E. Martín-Martínez, Work Distributions on Quantum Fields, Phys. Rev. Lett. **122**, 240604 (2019).

[53] A. Bartolotta and S. Deffner, Jarzynski Equality for Driven Quantum Field Theories, Phys. Rev. X **8**, 011033 (2018).

[54] P. Smacchia and A. Silva, Work distribution and edge singularities for generic time-dependent protocols in extended systems, Phys. Rev. E **88**, 042109 (2013).

[55] Z. Fei, J. Zhang, R. Pan, T. Qiu, and H. T. Quan, Quantum work distributions associated with the dynamical Casimir effect, Phys. Rev. A **99**, 052508 (2019).

[56] Z. Fei and H. T. Quan, Group-theoretical approach to the calculation of quantum work distribution, Phys. Rev. Research **1**, 033175 (2019).

[57] M. Scandi, H. J. D. Miller, J. Anders, and M. Perarnau-Llobet, Quantum work statistics close to equilibrium, Phys. Rev. Research **2**, 023377 (2020).

[58] A. D. Varizi, A. P. Vieira, C. Cormick, R. C. Drumond, and G. T. Landi, Quantum coherence and criticality in irreversible work, Phys. Rev. Research **2**, 033279 (2020).

[59] F. Liu, Derivation of quantum work equalities using a quantum Feynman-Kac formula, Phys. Rev. E **86**, 010103(R) (2012).

[60] Z. Fei, H. T. Quan, and F. Liu, Quantum corrections of work statistics in closed quantum systems, Phys. Rev. E **98**, 012132 (2018).

[61] Y. Qian and F. Liu, Computing characteristic functions of quantum work in phase space, Phys. Rev. E **100**, 062119 (2019).

[62] O. Brodier, K. Mallick, and A. M. O. de Almeida, Semiclassical work and quantum work identities in Weyl representation, J. Phys. A: Math. Theor. **53**, 325001 (2020).

[63] Z. Fei and H. T. Quan, Nonequilibrium Green's Function's Approach to the Calculation of Work Statistics, Phys. Rev. Lett. **124**, 240603 (2020).

[64] J.-J. Dong and Y. Yang, Functional field integral approach to quantum work, Phys. Rev. B **100**, 035124 (2019).

[65] C. Aron, G. Biroli, and L. F. Cugliandolo, (Non) equilibrium dynamics: A (broken) symmetry of the Keldysh generating functional, SciPost Phys. **4**, 008 (2018).

[66] J. Yeo, Symmetry and its breaking in a path-integral approach to quantum Brownian motion, Phys. Rev. E **100**, 062107 (2019).

[67] S. Montangero, *Introduction to Tensor Network Methods: Numerical Simulations of Low-Dimensional Many-Body Quantum Systems* (Springer, 2018).

[68] R. Orús, Tensor network for complex quantum systems, Nat. Rev. Phys. **1**, 538 (2019).

[69] M. Brenes, J. J. Mendoza-Arenas, A. Purkayastha, M. T. Mitchison, S. R. Clark, and J. Goold, Tensor-Network Method

to Simulate Strongly Interacting Quantum Thermal Machines, Phys. Rev. X **10**, 031040 (2020).

[70] M. Popovic, M. T. Mitchison, A. Strathearn, B. W. Lovett, J. Goold, and P. R. Eastham, Quantum Heat Statistics with Time-Evolving Matrix Product Operators, PRX Quantum **2**, 020338 (2021).

[71] S. Paeckel, T. Köhler, A. Swoboda, S. R. Manmana, U. Schollwöck, and C. Hubig, Time-evolution methods for matrix-product states, Ann. Phys. (NY) **411**, 167998 (2019).

[72] S. R. White, Minimally Entangled Typical Quantum States at Finite Temperature, Phys. Rev. Lett. **102**, 190601 (2009).

[73] M. Suzuki, Generalized Trotter's formula and systematic approximants of exponential operators and inner derivations with applications to many-body problems, Commun. Math. Phys. **51**, 183 (1976).

[74] D. Perez-Garcia, F. Verstraete, M. M. Wolf, and J. I. Cirac, Matrix product state representations, Quantum Inf. Comput. **7**, 401 (2007).

[75] E. M. Stoudenmire and S. R. White, Minimally entangled typical thermal state algorithms, New J. Phys. **12**, 055026 (2010).

[76] S. R. White, Density Matrix Formulation for Quantum Renormalization Groups, Phys. Rev. Lett. **69**, 2863 (1992).

[77] S. R. White, Density-matrix algorithms for quantum renormalization groups, Phys. Rev. B **48**, 10345 (1993).

[78] D. Andrieux and P. Gaspard, Quantum Work Relations and Response Theory, Phys. Rev. Lett. **100**, 230404 (2008).

[79] W. H. Press, S. A. Teukolsky, W. T. Vetterling, and B. P. Flannery, *Numerical Recipes. The Art of Scientific Computing*, 3rd ed. (Cambridge University Press, Cambridge, New York, 2007).

[80] T. H. Johnson, T. J. Elliott, S. R. Clark, and D. Jaksch, Capturing Exponential Variance using Polynomial Resources: Applying Tensor Networks to Nonequilibrium Stochastic Processes, Phys. Rev. Lett. **114**, 090602 (2015).

[81] B. Stroustrup, *The C++ Programming Language*, 4th ed. (Addison-Wesley, 2013).

[82] M. Fishman, S. R. White, and E. M. Stoudenmire, The itensor software library for tensor network calculations, arXiv:2007.14822.

[83] C. Psarras, L. Karlsson, J. Li, and P. Bientinesi, The landscape of software for tensor computations, arXiv:2103.13756.