Letter

Work statistics for the adiabatic assumption in nonequilibrium many-body theory

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Keldysh field theory, based on adiabatic assumptions, serves as a widely used framework for addressing nonequilibrium many-body systems. Nonetheless, the validity of such adiabatic assumption when addressing interacting Gibbs states remains a topic of contention. Interestingly, the knowledge of work statistics developed in nonequilibrium thermodynamics helps us to quantitatively explore this problem. Consequently, we deduce a universal theorem delineating the characteristics of evolutions that transition an initial Gibbs state to another. Based on this theorem, we analytically ascertain that adiabatic evolutions fail to transition a noninteracting Gibbs state to its interacting counterpart. However, the adiabatic evolution remains a superior approximation relative to its nonadiabatic counterparts. Numerics verifying our theory and predictions are also provided. Furthermore, our findings render insights into the Gibbs state preparation within the domain of quantum computation.

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Introduction. The concept of adiabatic driving has been widely used in quantum physics, including Berry phase [1], zero-temperature many-body theory [2,3], nonequilibrium many-body theory [4–6], and adiabatic quantum computation [7]. The adiabatic theorem [8–11] guarantees the validity of the adiabatic assumption in studying those physics. Specifically, in the zero-temperature many-body (field) theory, the Gell-Mann-Low theorem [2,3,12], which is a specialization of the adiabatic theorem for interacting many-body systems, indicates that one can obtain the interacting ground state from a noninteracting ground state by adiabatically switching on the interaction Hamiltonian. Such a reduction greatly facilitate the treatment of interacting systems, as it makes the noninteracting Green's functions as the building blocks.

Based on the Schwinger-Keldysh closed-time formalism [4,13,14], the nonequilibrium Green's functions serve as a useful framework for nonequilibrium many-body problems [5,15–19]. When considering nonequilibrium many-body systems, one is often staring from a Gibbs state at inverse temperature β, where the Hamiltonian is in the form of $H = H_0 + \lambda_1 H_1$ with H_1 being the interaction and λ_1 the interaction strength. To deal with such an interacting initial state, Konstantinov and Perel' [6,14] proposed that one can regard the interacting Gibbs state as an evolution in the imaginary time axis and then treat it with the imaginary time Matsubara formalism [20]. Despite the mathematical rigor of this approach, it presents complexities due to the concurrent handling of both imaginary-time and real-time Green's functions. Moreover, the treatment of interacting Gibbs states using Matsubara formalism is already a difficult task. Therefore, a streamlined formalism, predominantly focusing on real-time Green's functions for nonequilibrium many-body problems, is advantageous. To this end, Keldysh suggested an approach wherein the interacting Gibbs state is considered as the final state of an evolution that initiates from a noninteracting Gibbs state at $t = -\infty$, with interactions being adiabatically switched on [4–6]. Then, the building blocks reduce to noninteracting Green's functions and one only needs to concentrate on real times, as encountered in the zero-temperature many-body theory.

In contrast with the zero-temperature many-body theory, the validity of the adiabatic assumption within the nonequilibrium many-body framework remains an open question. Specifically, if an adiabatic evolution fails to transition a noninteracting Gibbs state to an interacting Gibbs state for a specified Hamiltonian [6,21], can the adiabatic assumption still be deemed a viable approximation when comparing with alternative evolution protocols? If the adiabatic assumption is a good approximation at finite temperature, then Keldysh approach can be still applied, which will definitely make treatments of nonequilibrium many-body problems more convenient due to the advantages of Keldysh approach. These heavily rely on analytical and quantitative descriptions of the accuracy of adiabatic assumption. In addition, the quantitative description also enables us to determine the regime in which the Keldysh approach fails. Furthermore, it is pertinent to explore the inherent characteristics of such evolution protocols capable of transitioning a noninteracting Gibbs state to its interacting counterpart. Insights from these properties might prove instrumental for Gibbs state preparation methodologies

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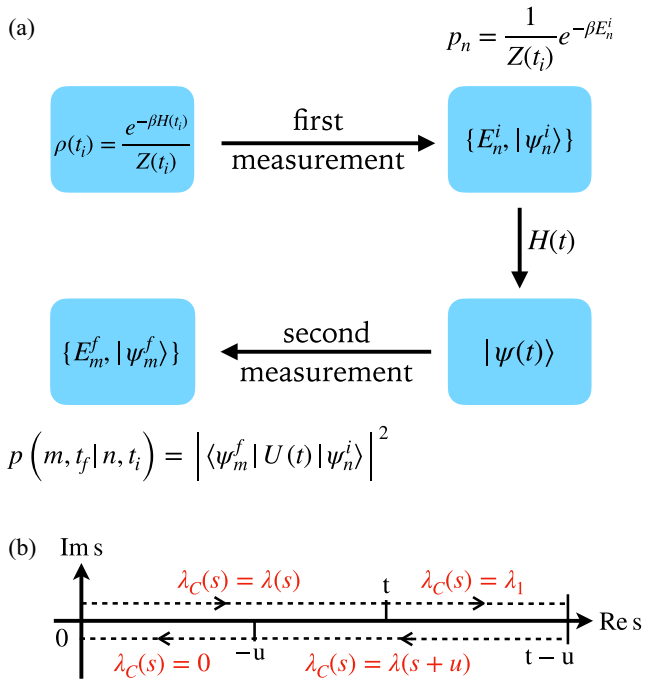

FIG. 1. (a) Definition of work statistics through two energy measurements. (b) The contour C used in calculating the characteristic function of work. The contour C is divided into four parts for our case: (i) $0 \to t$: $\lambda_C(s) = \lambda(s)$; (ii) $t \to t-u$ with $u < 0$: $\lambda_C(s) = \lambda_1$; (iii) $t-u \to t$: $\lambda_C(s) = \lambda(s+u)$; (iv) $-u \to 0$: $\lambda_C(s) = 0$.

[22–24]. In subsequent discussions, we refer to these evolution protocols as noninteraction-to-interaction (NI) evolution protocols.

In this work, we analytically and quantitatively discuss these problems, which becomes possible with the help of work statistics [25–32] developed in the nonequilibrium thermodynamics. Specifically, a universal theorem that holds for arbitrary quantum systems and determines the NI evolution protocol is derived. Generic calculations of work statistics show that the adiabatic evolution cannot transition a noninteracting Gibbs state to an interacting Gibbs state. However, comparing with nonadiabatic evolution protocols, the final state of the adiabatic evolution is closer to the desired interacting Gibbs state up to an error of the order of $O(\lambda_1^3)$. For nonadiabatic evolutions, the error is of the order of $O(\lambda_1^2)$.

Work statistics and Jarzynski equality. Before examining properties of the desired NI evolution protocol, we briefly review work statistics and the Jarzynski equality [25–33] within the context of quantum systems, as they enable us to quantitatively and universally consider those aforementioned problems.

Ingredients of work statistics in quantum version can be defined through two energy measurements [34,35] as shown in Fig. 1(a). In the first measurement, the energy outcome is determined by the initial Gibbs state $\rho(t_i) = e^{-\beta H(t_i)}/Z(t_i)$ with $Z(t_i) = \mathrm{tr}[e^{-\beta H(t_i)}]$ being the partition function of the initial system. The first measurement can produce an eigenvalue E_n^i of $H(t_i)$ with a probability $p_n = e^{-\beta E_n^i}/Z(t_i)$. Subsequent to this, the system transitions to the eigenstate $|\psi_n^i\rangle$ and evolves according to the time-dependent Hamiltonian $H(t)$ under the unitary evolution $U(t)$. At the final time t_f, another measurement results in the eigenvalue E_m^f of $H(t_f)$ with a conditional probability $p(m, t_f|n, t_i) = |\langle\psi_m^f|U(t_f)|\psi_n^i\rangle|^2$. Here, $|\psi_m^f\rangle$ signifies the eigenstate of $H(t_f)$ corresponding to E_m^f. Consequently, the joint probability of obtaining measurements E_m^f and E_n^i is $p(m, t_f|n, t_i)p_n$. The work is defined as the difference of two energy outcomes: $w = E_m^f - E_n^i$, and the probability of work w should be

$$p(w) = \sum_{n,m} \delta\left[w - \left(E_m^f - E_n^i\right)\right] p(m, t_f|n, t_i) p_n. \tag{1}$$

Having derived the work distribution, one can also define the characteristic function of work (CFW) through the Fourier transformation of $p(w)$:

$$\begin{aligned}\chi(u) &= \int dw e^{iuw} p(w) \\ &= \frac{1}{Z(t_i)} \mathrm{tr}\left[U^\dagger(t_f) e^{iuH(t_f)} U(t_f) e^{-(iu+\beta)H(t_i)}\right].\end{aligned} \tag{2}$$

The CFW is a more convenient tool in studying nonequilibrium physics of quantum systems than the distribution $p(w)$. Remarkably, by setting $u = i\beta$ in the CFW, one can obtain the Jarzynski equality [25]:

$$\langle e^{-\beta w}\rangle = \frac{Z(t_f)}{Z(t_i)}, \tag{3}$$

where $\langle\cdot\rangle$ without subscript is defined as $\langle\cdot\rangle = \int dw(\cdot)p(w)$, and $Z(t_f) = \mathrm{tr}[e^{-\beta H(t_f)}]$ is the partition function of a *hypothetical* system with Hamiltonian $H(t_f)$ in a Gibbs state at inverse temperature β. Note that the real system at t_f is not necessarily at a Gibbs state. Hence, it is also desirable to ask that when the real system will be in a Gibbs state at t_f.

Properties of the noninteraction-to-interaction evolution protocol. In the following, we present the theorem elucidating the properties of the noninteraction-to-interaction (NI) evolution protocol. Prior to that, we introduce two lemmas essential for the proof of the theorem. We provide only a succinct overview of the pivotal steps in the proof, with comprehensive details available in the Supplemental Material (SM) [36].

Lemma 1. The averaged work $\langle w\rangle \equiv \int dw w p(w)$ of an evolution from t_i to t_f, can also be expressed as $\langle w\rangle = \langle H(t_f)\rangle_{t_f} - \langle H(t_i)\rangle_{t_i}$, where $\langle H(t)\rangle_t \equiv \mathrm{tr}[\rho(t)H(t)]$.

Lemma 2. Suppose there exists an evolution protocol from t_i to t_f, such that for all systems, the average work of the evolution satisfies $\langle w\rangle = \langle H(t_f)\rangle_G - \langle H(t_i)\rangle_{t_i}$, where

$$\langle H(t_f)\rangle_G \equiv \frac{1}{\mathrm{tr}\left[e^{-\beta H(t_f)}\right]} \mathrm{tr}\left[e^{-\beta H(t_f)} H(t_f)\right],$$

then the final state $\rho(t_f)$ is a Gibbs state with respect to $H(t_f)$ at inverse temperature β.

Having derived the above two lemmas, we are now able to prove a theorem, which gives the property of the desired evolution protocol for arbitrary systems.

Theorem 1. For any given system with an initial Hamiltonian $H(t_i)$ and a final Hamiltonian $H(t_f)$, an evolution that drives the initial Gibbs state $\rho(t_i) = e^{-\beta H(t_i)}/Z(t_i)$ to the final one $\rho(t_f) = e^{-\beta H(t_f)}/Z(t_f)$, exists *if and only if* the work distribution $p(w)$ is a δ function.

Proof.

(a) We first prove the sufficiency. If the work distribution is $p(w) = \delta(w - w_0)$ (for different systems, w_0 can be different), then the work of each trajectory should be the same, and equals to the average $\langle w \rangle$. According to the Jarzynski equality Eq. (3), one has

$$\langle e^{-\beta w} \rangle = e^{-\beta w_0} = \frac{Z(t_f)}{Z(t_i)}, \tag{4}$$

where $Z(t_f)$ is the partition function of a *hypothetical* system with Hamiltonian $H(t_f)$ in a Gibbs state at inverse temperature β. Then

$$\langle w \rangle = -\frac{\partial}{\partial \beta} \ln \frac{Z(t_f)}{Z(t_i)} = \langle H(t_f) \rangle_G - \langle H(t_i) \rangle_{t_i}. \tag{5}$$

According to Lemma 2, we know that the state of the *real* system at t_f is the Gibbs state $\rho(t_f) = e^{-\beta H(t_f)}/Z(t_f)$.

(b) We next prove the necessity. If the state at t_f is $\rho(t_f) = e^{-\beta H(t_f)}/Z(t_f)$, then according to Lemma 1, one has

$$\langle w \rangle = \langle H(t_f) \rangle_{t_f} - \langle H(t_i) \rangle_{t_i} = -\frac{\partial}{\partial \beta} \ln \frac{Z(t_f)}{Z(t_i)}. \tag{6}$$

In addition, the Jarzynski equality will lead to

$$-\frac{\partial}{\partial \beta} \ln \langle e^{-\beta w} \rangle = -\frac{\partial}{\partial \beta} \ln \frac{Z(t_f)}{Z(t_i)}. \tag{7}$$

Combining Eqs. (6) and (7), one has

$$\langle w \rangle = -\frac{\partial}{\partial \beta} \ln \langle e^{-\beta w} \rangle \Rightarrow \quad \langle w e^{-\beta w} \rangle = \langle w \rangle \langle e^{-\beta w} \rangle. \tag{8}$$

In order that Eq. (8) holds, w and $e^{-\beta w}$ must be independent or the trajectory work w is a constant. Since both of w and $e^{-\beta w}$ are functions of w, they must not be independent. Therefore, Eq. (8) requires that the trajectory work w should be a constant, that is $w = w_0$, where w_0 is a constant but can be different for different systems. Therefore, the work distribution for the desired evolution protocol should be a δ function,

$$p(w) = \delta(w - w_0). \tag{9}$$

■

The time-independent case is a trivial example of this theorem. In this case, the final Gibbs state is identical with the initial Gibbs state, and the state after the first measurement only acquires a overall phase under the evolution provided by the time-independent Hamiltonian. Thus the trajectory work is simply $w = w_0 = 0$.

Given the utility of the characteristic function of work (CFW) in facilitating analysis, we derive a corollary based on Theorem 1 in order to capture the property through the CFW.

Corollary 1. The logarithm of the characteristic function of work $\chi(u)$ for the evolution protocol given by Theorem 1 satisfies $\ln \chi(u) = iuw_0$, where w_0 is a real number.

Here, we would like to emphasize again that we are not researching some problems exiting in the field of nonequilibrium thermodynamics, but just apply the knowledge of nonequilibrium thermodynamics to consider the foundation of Keldysh field theory. One may ask why we have to use work statistics to consider the problem. The reason is that, to our knowledge, other approaches like calculating traditional observable expectations in quantum mechanics and perturbatively treating the equation of motion, cannot give us analytical and quantitative information if we would like to universally treat this problem without depending on specific models.

Perturbative calculations of the characteristic function of work. For systems under an arbitrary nonequilibrium evolution, computing the CFW can be challenging. Nonetheless, when the full interaction strength, denoted λ_1 in the Hamiltonian $H = H_0 + \lambda_1 H_1$, is small, a universal formula for the CFW can be derived via the perturbation theory [35]. Given the suitability of field theory techniques to weakly interacting quantum many-body systems, our focus predominantly lies within the perturbative domain.

Given the time evolution protocol where the interaction is gradually turned on from zero to t, the exponential operators in Eq. (2) can all be treated as evolution operators along either real-time axis or imaginary-time axis. Thus, analogous to the Schwinger-Keldysh contour, the CFW can be written in a contour-integral form [35]:

$$\chi(u) = \left\langle \mathcal{T}_C \left[e^{-i \int_C ds \lambda_C(s) H_1^I(s)} \right] \right\rangle_0, \tag{10}$$

where $\langle \cdot \rangle_0 = \mathrm{tr}[(\cdot) e^{-\beta H_0}]/\mathrm{tr}[e^{-\beta H_0}]$, $\mathcal{T}_C$ is the contour-ordered operator with C being the contour analogous to the Schwinger-Keldysh contour, and $H_1^I(s) = e^{iH_0 s} H_1 e^{-iH_0 s}$ is the interacting Hamiltonian in the interaction picture. The contour is divided into four parts as shown in Fig. 1(b), according to the value of $\lambda_C(s)$. As the initial interaction strength is zero, the contour only resides on the real-time axis.

The logarithm of $\chi(u)$, known as cumulant CFW, can be expanded via cumulant correlation functions [35,37]:

$$\ln \chi(u) = \sum_{n=1}^{\infty} \int_C d\bar{s}_1 \cdots d\bar{s}_n G_c(s_1, \ldots, s_n), \tag{11}$$

where $d\bar{s}_l \equiv ds_l \lambda_C(s) \theta_C(s_l - s_{l+1})$ with $\theta_C(s_l - s_{l+1})$ being the contour step function [35] and $\theta_C(s_n - s_{n+1}) \equiv 1$, and $G_c(s_1, \ldots, s_n) \equiv (-i)^n \langle H_1^I(s_1) \cdots H_1^I(s_n) \rangle_c$ is the n-point cumulant correlation function.

For nonadiabatic evolutions in our case, $\ln \chi(u)$ up to second order of λ_1 is given by

$$\ln \chi(u) = iu\lambda_1 \langle H_1 \rangle_c + iu\lambda_1^2 \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{G_c^>(\omega)}{\omega} + \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{1 - e^{i\omega u}}{\omega^2} A(\omega) G_c^>(\omega) + O(\lambda_1^3), \tag{12}$$

where $G_c^>(\omega)$ is the Fourier transformation of $G_c^>(s_1 - s_2) \equiv G_c(s_1, s_2)$, and $A(\omega) \equiv |\int_0^t ds \dot{\lambda}(s) e^{i\omega s}|^2$. It is easy to verify that $G_c^>(\omega)$ is a real function, the first and second term match Corollary 1, while the third term does not. For the adiabatic case, $t \to \infty$ and $\dot{\lambda}(s) \to 0$, then the third term containing $A(\omega)$ approaches zero. Thus, for adiabatic cases, $\ln \chi(u)$ is linear in u when we keep terms up to $O(\lambda_1^2)$, and then matches our theorem (or corollary). To see whether this holds for arbitrary order, we calculate $\ln \chi(u)$ up to $O(\lambda_1^3)$ for the adiabatic

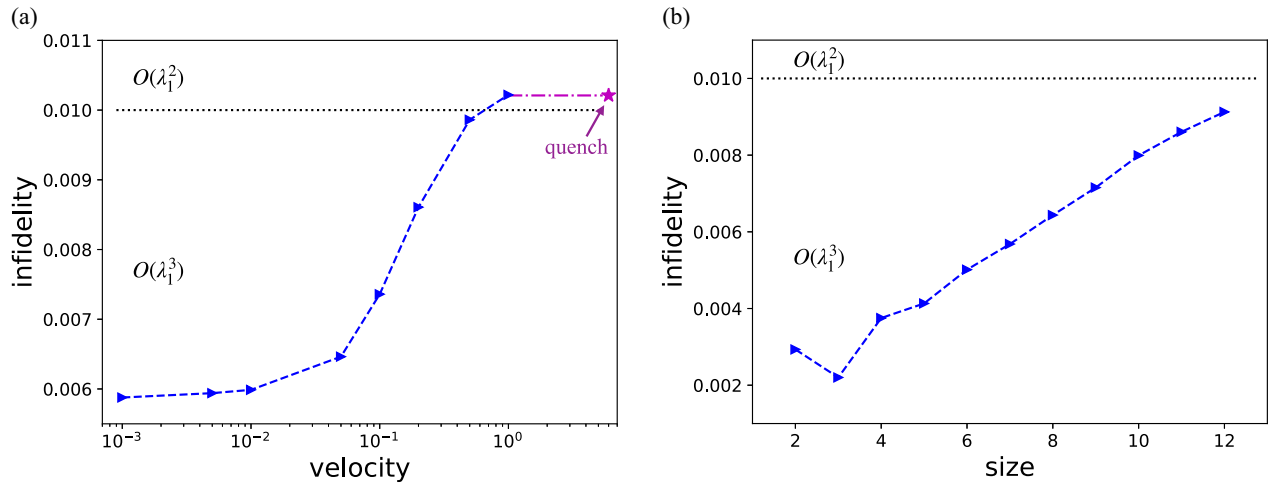

FIG. 2. Infidelities (1 − fidelity) between the interacting Gibbs state and final states of different evolution protocols. The parameters in common are chosen to be $J = 2$, $\lambda_1 = 0.1$, $\beta = 1$. The total time for each evolution is $\lambda_1/0.001 = 100$. (a) Infidelities for different evolution velocities of the linear driving $\lambda(t) = vt$. The size of the XXZ chain is chosen to be $N = 11$. The final point marked as a star represents the quench evolution protocol, the velocity of which is regarded as ∞. For velocities larger than 0.001, the system will reach the full interaction before $t = 100$, and then the system will continue to evolve with full interaction until time reaches 100. (b) Infidelities for different sizes of the XXZ chain. The increasing velocity is chosen to be $v = 0.2$ and the evolution time is also $t = 100$.

case and obtain

$$\ln \chi(u) = iu\lambda_1 \langle H_1 \rangle_c + iu\lambda_1^2 \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{G_c^>(\omega)}{\omega} + iu\lambda_1^3 \int_{-\infty}^{\infty} \frac{d\omega_1}{2\pi} \frac{d\omega_2}{2\pi} \frac{G_c^>(\omega_1, \omega_2)}{i\omega_1(\omega_1 + \omega_2)} + O(\lambda_1^4), \tag{13}$$

where $G_c^>(\omega_1, \omega_2)$ is the Fourier transformation of $G_c^>(s_1 - s_3, s_2 - s_3)$, which is defined as

$$\begin{aligned} &G_c^>(s_1 - s_3, s_2 - s_3) \\ &\quad \equiv (-i)^3 \left\langle H_1^I(s_1 - s_3) H_1^I(s_2 - s_3) H_1^I(0) \right\rangle_c \\ &\quad = G_c(s_1, s_2, s_3). \end{aligned} \tag{14}$$

One finds that $O(\lambda_1^3)$ term does not match Corollary 1, as one can demonstrate that $G_c^>(\omega_1, \omega_2)$ is a complex function. Complete calculations can be found in the SM [36].

Upon examining the universal criteria set by Theorem 1 (Corollary 1), we discern that neither adiabatic nor nonadiabatic evolution protocols can transition a noninteracting Gibbs state to its interacting counterpart (see the SM [36] for an intuitive interpretation). Notably, the logarithmic CFW for adiabatic protocols deviates from that of the NI protocol (shown in Corollary 1) to the order of $O(\lambda_1^3)$, while for nonadiabatic protocols, the discrepancy occurs to the order of $O(\lambda_1^2)$ [evident from the third term in Eq. (12)]. This suggests that although adiabatic evolution does not precisely achieve the desired state transition, it offers a superior approximation relative to nonadiabatic alternatives.

Numerical verification. The former discussions are general and universal without depending on specific models in order to verify our theory and the prediction of accuracy of the adiabatic assumption, we consider numerical results for a specific model—one-dimensional XXZ spin chain. The Hamiltonian reads

$$H_{xxz} = J \sum_{i=1}^{N-1} \left[\sigma_i^+ \sigma_{i+1}^- + \sigma_{i+1}^- \sigma_i^+ + \lambda(t) \sigma_i^z \sigma_{i+1}^z \right], \tag{15}$$

where $\lambda(t)$ controls the zz interaction strength. For a given model, to check whether these two states are identical, one can directly compute the fidelity [38] between the interacting Gibbs state and the final state after an evolution. Without loss of generality, we consider a linear driving protocol $\lambda(t) = vt$, where v is the increasing velocity of the interaction strength. For a given system size, an evolution with larger v is more nonadiabatic. We consider the small interaction regime, in which our perturbative calculation works. We finally arrive at Fig. 2(a). One finds that larger velocities will lead to a final state more deviated from the target interacting Gibbs state. This confirms the result of our universal analysis based on work statistics. Remarkably, in the nearly adiabatic regime (small v), the infidelity is approximately the order of $O(\lambda_1^3)$, while in the nonadiabatic regime (large v), the infidelity (1-fidelity) is the order of $O(\lambda_1^2)$. This result matches the prediction based on the logarithmic CFW. For smaller sizes with identical J and λ, energy gaps will be larger, thus for a fixed increasing velocity, the evolution will be more adiabatic, and one is expected to see smaller infidelities. This argument is confirmed by Fig. 2(b). In addition, the infidelity in the adiabatic regime is still the order of $O(\lambda_1^3)$.

Conclusion. In summary, based on work statistics, we derived a theorem elucidating the thermodynamic properties of an evolution transitioning an initial Gibbs state to another one. In the realm of weak interactions, where the Keldysh field theory becomes particularly applicable, our theorem analytically demonstrates that the adiabatic evolution does not precisely transition a noninteracting Gibbs state to its interacting counterpart. Nevertheless, in this work, we analytically show that when contrasted with nonadiabatic protocols, the resultant state from adiabatic evolution presents a closer approximation

to the desired interacting Gibbs state. Our numerical simulation confirms the theoretical prediction.

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