Relations between dissipated work in non-equilibrium process and the family of Rényi divergences

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Abstract

In this paper, we establish a general relation which directly links the dissipated work done on a system driven arbitrarily far from equilibrium, a fundamental quantity in thermodynamics, and the family of Rényi divergences between two states along the forward and reversed dynamics, a fundamental concept in information theory. Specifically, we find that the generating function of the dissipated work under an arbitrary time-dependent driving is related to the family of Rényi divergences between a non-equilibrium state along the forward process and a non-equilibrium state along its time-reversed process. This relation is a consequence of the principle of conservation of information and time reversal symmetry and is universally applicable to both finite classical system and finite quantum system under arbitrary driving process. The significance of the relation between the generating function of dissipated work and the family of Rényi divergences are two fold. On the one hand, the relation establishes that the macroscopic entropy production and its fluctuations are determined by the family of Rényi divergences, a measure of distinguishability of two states, between a microscopic process and its time reversal. On the other hand, this relation tells us that we can extract the family of Rényi divergences from the work measurement in a microscopic process. For classical systems the work measurement is straightforward, from which the family of Rényi divergences can be obtained; for quantum systems under time-dependent driving the characteristic function of work distributions can be measured from Ramsey interferences of a single spin, then we can extract the family of Rényi divergences from RAMsey interferences of a single spin.

1. Introduction

The pioneering works by Clausius and Kelvin have established that the average mechanical work needed to move a system in contact with a heat bath at temperature $T$, from one equilibrium state $A$ into another equilibrium state $B$, is at least equal to the free energy difference between these states: $\langle W \rangle \geq F_B - F_A$, where the equality holds only for a quasi-static process. In a remarkable development Jarzynski [1] discovered that for a classical system initialized in an equilibrium state the work done under a non-equilibrium change of control parameters is related to the equilibrium free energy difference between the initial and the final equilibrium states for the control parameters via

$$\langle e^{-\beta W} \rangle = \frac{Z(\beta, \lambda_f)}{Z(\beta, \lambda_i)} = e^{-\beta[F(\beta, \lambda_f) - F(\beta, \lambda_i)]}$$

Here $\beta \equiv 1/T$ is the inverse temperature $T$ of the initial equilibrium state of the system and we take the Boltzmann constant $k_B \equiv 1$, $W$ is the work done on the system due to a driving protocol which varies the control parameter from $\lambda_i$ to $\lambda_f$, $F \equiv -\beta^{-1} \ln Z$ is the Helmholtz free energy of the system with $Z$ being the equilibrium partition function and the angular bracket on the left of equation (1) denotes an ensemble average over realizations of the process. The Jarzynski equality connects equilibrium thermodynamic quantity, the free energy difference, to a non-equilibrium quantity, the work done in an arbitrary driving processes. It implies that
we can determine the equilibrium free energy difference of a system by repeatedly performing work at any rate. Jarzynski equality and Crooks relation \[ \] from which it can be derived have been verified experimentally in various physical systems \[ \] and were also proven to hold for finite quantum mechanical systems \[ \]. The discovery of the Jarzynski equality has led to a very active field concerned with fluctuation relations in non-equilibrium thermodynamics \[ \].

The excess work \( W - \Delta F \) that arises in irreversible processes is often referred to as the dissipated work, \( W_{\text{diss}} = W - \Delta F \). Contrary to the reversible work, which only depends on the initial and final equilibrium states, the dissipated work depends on how the specific driven protocol is performed. Usually the driving protocol is realized by changing the control parameters in the Hamiltonian between initial and final values, which can in principle bring the system arbitrarily far out of equilibrium. Surprisingly, there exists a neat and exact microscopic fluctuation relation for the dissipated work. The central result of this paper is the following relation:

\[
\langle e^{-\beta W_{\text{diss}}} \rangle = e^{\lambda_2 t} \langle \Psi_{\text{diss}}(\lambda_2 \tau t) | \psi(t) \rangle, \tag{2}
\]

where \( z \) is a real number, \( W_{\text{diss}} \) is the dissipated work done on the system due to a driving protocol under which the control parameter changes from \( \lambda_i \) to \( \lambda_f \), the angular bracket on the left hand side denotes an ensemble average over the realizations of the driving process and \( S_z \left[ \Theta \rho_\beta (\tau - t) \Theta^{-1} | \rho_\beta (t) \right] \) is the order-\( z \) Rényi divergence between \( \Theta \rho_\beta (\tau - t) \Theta^{-1} \) and \( \rho_\beta (t) \) with \( \Theta \) being the time reversal operation. For classical system, the order-\( z \) Rényi divergence between two distributions \( \rho_\beta (X) \) and \( \rho_\beta (X) \) is defined as \( S_z[\rho_\beta (X) | \rho_\beta (X)] \equiv \frac{1}{z-1} \ln \int dX \rho_\beta^z (X) \rho_\beta^{1-z} (X) \), \( \rho_\beta (t) \) is the phase space density in the forward process at an arbitrary time \( t \in [0, \tau] \) which is initialized in an equilibrium state at inverse temperature \( \beta \) and control parameter \( \lambda_i \) and \( \rho_\beta (\tau - t) \) is the phase space density in the reversed process at time \( \tau - t \) which is initialized in an equilibrium state at inverse temperature \( \beta \) and control parameter \( \lambda_f \). For quantum system, the order-\( z \) Rényi divergence between quantum states \( \rho_\beta \) and \( \rho_\beta \) is defined as \( S_z[\rho_\beta | \rho_\beta] \equiv \frac{1}{z-1} \ln \text{Tr} [\rho_\beta^z \rho_\beta^{1-z}] \), \( \rho_\beta (t) \) is the density matrix in the forward process at arbitrary time \( t \in [0, \tau] \) which is initialized in the canonical equilibrium state at inverse temperature \( \beta \) and force parameter \( \lambda_i \) and \( \rho_\beta (\tau - t) \) is the density matrix at time \( \tau - t \) in the time reversed process which was initialized in the canonical equilibrium state at inverse temperature \( \beta \) and force parameter \( \lambda_f \). It should be emphasized that because of the assumption that the system is isolated from the reservoir before and in the course of driven, the right hand side of equation (2) can be written as the Rényi divergence between the state of the forward process and the state of backward process at same time \( \tau \) while in the case of an open system the probabilities of the entire process may appear. Equation (2) can be consider as a generalization of Jarzynski equality in equation (1) and includes Jarzynski equality as a special case. Jarzynski equality states that average of \( e^{-\beta W} \) on the work distribution measurement gives the free energy difference between the equilibrium states at the initial and final parameters. We are attempting to explore whether work distribution in a non-equilibrium driving can produce more knowledge about the physical process and physical system than that of Jarzynski equality tells us. Equation (2) is a useful result in this direction.

The remainder of this paper is organized as follows: in section 2, we briefly review the formalism for non-equilibrium classical thermodynamics, including the concept of work in classical system, the forward driving process and its time reversed process and then derive the relation between the generating function of dissipated work and the family of Rényi divergences between two phase space distributions along the forward and reversed process. In section 3, we review the formalism for quantum thermodynamics and then derive the relations between the generating function of dissipated work in driven quantum system and the family of Rényi divergences between two quantum states along the forward and its time reversed process. In section 4, we establish the formalism for extracting the family of Rényi divergences for two quantum states from the Ramsey interference of a single spin. In section 5 we use the one-dimensional (1D) transverse field Ising model in a sudden quench process to demonstrate our theoretical finding, equation (2), between the generating function of dissipated work and the family of Rényi divergences between two quantum states and then we use a single spin undergoing a sudden quench process to demonstrate the method of extracting the family of Rényi divergences from the Ramsey interference of a single spin. In section 6, we summarize our findings and discuss the possible related future problems.

2. Non-equilibrium classical thermodynamics

We consider a finite classical system with Hamiltonian \( H \{ X; \lambda \} \), where \( X = \{ q_1, p_1; q_2, p_2; \ldots; q_N, p_N \} \) denotes collectively the coordinates and momenta of all the \( N \) particles in the system, \( \lambda \) is a parameter controlled by an external agent. For a classical system with time-dependent Hamiltonian, the microscopic reversibility \[ \] is illustrated in figure 1.

We first introduce the forward process for a classical system under time-dependent driving. We assume that the classical system is initialized in the equilibrium state at inverse temperature \( \beta = 1/T \) with the control...
Here, the parameter $\lambda$, which is described by the Boltzmann distribution in phase space $\rho_0[X; 0] = e^{-\beta H[X; \lambda]} / Z(\beta, \lambda)$ with $Z(\beta, \lambda) = \int dX_0 e^{-\beta H[X_0; \lambda]}$ being the initial partition function. Then the classical system is isolated and driven by an external agent, which varies the control parameter $\lambda$ from an initial value $\lambda_0$ to a final value $\lambda_f$ in a time duration $\tau$ according to a specified protocol $\lambda(t)$, $t \in [0, \tau]$. According to Liouville theorem, which states that the phase space distribution is invariant along any trajectory of the system [25], one has, for $\forall t \in [0, \tau]$,

$$\rho_0[X(t); t] = \rho_0[X_0; 0],$$

where $X(t)$ is the resulting phase space point at time $t$ under the dynamics of forward Hamiltonian $H[X; \lambda(t)]$ if it was initially at $X_0$ at $t = 0$ (see the upper red line in figure 1). According to first law of thermodynamics, the work done associated with the trajectory in the forward process is

$$W[X_0] = H[X_0; \lambda_0] - H[X_0; \lambda_1].$$

Now we consider the reversed process. In the reversed process, the classical system is initialized in a canonical equilibrium state at inverse temperature $\beta$ at the value $\lambda_f$ of the control parameter,

$$\rho_f[X; 0] = e^{-\beta H[X; \lambda_f]} / Z(\beta, \lambda_f) = \Theta e^{-\beta H[X; \lambda_f]} \Theta^{-1} / Z(\beta, \lambda_f)$$

with $Z(\beta, \lambda_f) = \int dX e^{-\beta H[X; \lambda_f]}$. Then the classical system is completely isolated and driven by the reversed Hamiltonian $H_R[X; t] = \Theta H[X; \lambda(\tau - t)] \Theta^{-1}$, $t \in [0, \tau]$ for a time duration $\tau$. According to Liouville theorem [25], we have

$$\rho_f[\Theta X(\tau - t); t] = \rho_f[\Theta X_0; 0].$$

Here $\Theta X(\tau - t)$ is the resulting phase space point at time $t$ under the dynamics of Hamiltonian in the reversed process $H_R[X; t]$ if it was at $\Theta X_0$ at $t = 0$ (see the lower blue line in figure 1).

Combining equations (3), (4) and (5), we obtain [26]

$$e^{-\beta(W - \Delta F)} = \frac{\rho_f[\Theta X(t); \tau - t]}{\rho_f[X(t); t]} = \frac{\Theta \rho_f[X(t); \tau - t] \Theta^{-1}}{\rho_f[X(t); t]},$$

where $\Delta F \equiv F[\beta, \lambda_f] - F[\beta, \lambda_0]$, with $F[\beta, \lambda] \equiv -\beta^{-1} \ln Z[\beta, \lambda]$ being the Helmholtz free energy, $t \in [0, \tau]$ is arbitrary time points. Note that on the right hand side of equation (6), the phase space densities are observed at the same phase space point $X(t)$. Equation (6) is a consequence of Liouville theorem in classical mechanics.

Making use of equation (6), we have

$$\langle e^{-\beta W} \rangle_F = \int dX_0 \rho_0[X_0; 0] e^{-\beta W[X_0]},$$

$$= e^{-\beta \Delta F} \int dX \rho_f[X; t] \left( \frac{\rho_f(\Theta X; \tau - t)}{\rho_f[X; t]} \right)^\gamma,$$

where $\gamma$ is the thermostat parameter.
\[ e^{-\beta s} \int dX \rho_k(X; t) \rho_k(\Theta X; \tau - t)^2, \]  
\[ e^{-\beta s} e^{(\tau - 1) \beta} \rho_k(X; \tau - t) \]  
\[ S_2 \rho_k(\Theta X; \tau - t) \rho_k(X; t), \]  
where \( s \) is a real finite number and \( S_2 = \frac{1}{2} \ln \left[ \int dX \rho_k(X) \rho_k(X)^2 \right] \) is the order-2 Rényi divergence of two probability distributions \( \rho_k(X) \) and \( \rho_k(\Theta X; \tau - t) \). From equations (7) to (8) we have applied the Liouville theorem \( dX = dX_0 \) and equation (6). Identifying the dissipated work \( W_{\text{diss}} = W - \Delta F \) in equations (7) to (10), we consequently obtain equation (2) for a classical system. Now we give several comments on equation (2) for classical system:

1. For \( z = 1 \), equation (2) for driven classical system returns to the Jarzynski equality [1] for classical system.
2. The fluctuation of the dissipated work is independent of time \( t \) because the densities on equation (10) can be evaluated at any intermediate time. While the fact that the dissipated work is independent of \( t \) can also be seen from [26, 29]. This time independence is a consequence of the Liouville equation in Hamilton dynamics.
3. For \( 0 < z < 2 \), the Rényi divergence for any two probability distributions \( \rho_1 \) and \( \rho_2 \) and any classical channel \( \varepsilon \) satisfies [21]

\[ S_z [\varepsilon (\rho_1), \varepsilon (\rho_2)] \leq S_z [\rho_1, \rho_2]. \]  
Therefore the Rényi divergence for \( 0 < z < 2 \) is a valid measure of distinguishability. Thus the family of Rényi divergences appears in equation (2) for classical system is a quantification of the breaking of time reversal symmetry between the forward process and its time reversed one.
4. It relates the fluctuation of dissipated work or entropy production to the family of Rényi divergences between the phase space density in the forward process and the phase density in its reversed process. Entropy production is a macroscopic quantity while the Rényi divergences between two states is essentially a microscopic quantity, which quantifies the distance between two states or to what extent the time reversal symmetry is breaking. The various moments of the dissipated work are given by,

\[ \langle W_{\text{diss}}^n \rangle = T^n \int dX \rho_k(X; t) \left( \ln \frac{\rho_k(X; t)}{\rho_k(\Theta X; \tau - t)} \right)^n, \]  
where \( n = 1, 2, 3, \ldots \) and \( T \) is the temperature. In particular for \( n = 1 \), the mean of the dissipation is [26–30]

\[ \langle W_{\text{diss}} \rangle = D[\rho_k(X; t) || \rho_k(\Theta X; \tau - t)], \]  
where \( D[\rho_k(X; t) || \rho_k(\Theta X; \tau - t)] \) is the relative entropy [31] between forward phase space density distributions and the reversed phase space density distributions.
5. It is an exact relation between the generating function of the dissipated work in a driving process and the family of Rényi divergences between two non-equilibrium states. Work distributions has been measured in various classical systems [3–5, 16, 17], from which one can extract the family of Rényi divergences between two classical phase space densities along the forward and reversed process.

3. Non-equilibrium quantum thermodynamics

Let us consider a finite quantum system governed by a Hamiltonian \( H(\lambda) \) and \( \lambda \) is a parameter controlled by an external agent. We illustrate the time reversal symmetry for quantum system under time-dependent driving in figure 2.

Let us first define the forward process in quantum system under time-dependent driving. We initialize the quantum system in canonical equilibrium state at inverse temperature \( \beta = 1/T \) at a fixed value of control parameter \( \lambda_0 \), which is described by the density matrix \( \rho_0(t) = e^{-\beta H(\lambda_0)} / Z(\lambda_0) \) with \( Z(\lambda) = \text{Tr}[e^{-\beta H(\lambda)}] \) being the partition function. Then we isolate the system and drive it by the Hamiltonian \( H(\lambda(t)) \) for a time duration \( \tau \), where the force protocol \( \lambda(t) \), \( t \in [0, \tau] \) brings the parameter from \( \lambda_0 \) at \( t = 0 \) to \( \lambda_0 \) at a later time \( \tau \). Then the state at \( t \) in the forward process is given by

\[ \rho_F(t) = U_F(t, 0) \rho_0(0) U_F^\dagger(t, 0), \]  
where \( U_F(t, 0) = T e^{\int_0^t d\tau H(\lambda(\tau))} \) with \( T \) being the time ordering operator. In general \( \rho_F(\tau) \) is different from the canonical equilibrium state \( \rho_k(\Theta X; \tau - t) \) of the quantum system defined by two projective measurements [14, 18]. We assume, for any \( \lambda, H(\lambda) | n(\lambda) \rangle = E_n(\lambda) | n(\lambda) \rangle \) and the symbol \( n \) labels
eigenenergy. At \( t = 0 \), the first projective measurement of \( H(\lambda_t) \) is performed with outcome \( E_\ell(\lambda_t) \) with probability \( p_{\ell,0}(0) = e^{-\beta E_\ell(\lambda_t)}/Z(\beta, \lambda_t) \). Simultaneously the initial equilibrium state projects into the state \( |n(\lambda_t)\rangle \). At \( 0 < t < \tau \), the system is isolated and driven by a unitary evolution operator \( U_\ell(t, 0) \) and the state at \( \tau \) is \( U_\ell(\tau, 0)|n(\lambda_t)\rangle \). At \( t = \tau \), the second projective measurement of \( H(\lambda_t) \) yielding the eigenvalue \( E_m(\lambda_t) \) with conditional probability \( p_{m|\ell,n}(\tau) = |\langle m(\lambda_t)|U_\ell(\tau, 0)|n(\lambda_t)\rangle|^2 \) is performed. So the probability of obtaining \( E_m(\lambda_t) \) for the first measurement and followed by obtaining \( E_m(\lambda_t) \) in the second measurement is \( p_{\ell,0}(0)p_{m|\ell,n}(\tau) \). Thus the work distribution in the forward process is given by \( [14, 18] \)

\[
P_f(W) = \sum_{m,n} p_{\ell,0}(0)p_{m|\ell,n}(\tau) \delta[W - E_m(\lambda_t) + E_n(\lambda_t)].
\]

The quantum work distribution \( P_f(W) \) encodes the fluctuations in the work that arise from thermal statistics and from quantum measurement statistics over many identical realizations of the protocol. The characteristic function of quantum work distribution is given by

\[
G(u) = \int_{-\infty}^{\infty} dW P_f(W)e^{iuW},
\]

\[
= Z(\beta, \lambda_t)^{-1} \text{Tr}[U(\tau)e^{-\beta H}e^{-iuH}U^\dagger(\tau)e^{iuH}].
\]

Now we define the **reversed process in quantum system**. In the reversed process, we initialize the quantum system in the time reversed state of the canonical equilibrium state at inverse temperature \( \beta = 1/T \) at value \( \lambda_t \) of the control parameter, \( \rho_R(0) = \Theta e^{-\beta H(\lambda_t)}\Theta^{-1}/Z(\beta, \lambda_t) \) with \( Z(\beta, \lambda_t) = \text{Tr}[e^{-\beta H(\lambda_t)}] \) being the canonical partition function. Then we drive the system by the Hamiltonian in the reversed process \( H_R(t) = \Theta H(\lambda(\tau - t))\Theta^{-1} \) for a time duration \( \tau \) which brings the force parameter from \( \lambda_t \) at \( t = 0 \) to \( \lambda_t \) at a later time \( \tau \). The time evolution operator for the forward process and its the reversed process are related by \([32]\)

\[
U_R(t, 0) = \Theta U^\dagger_f(\tau, \tau - t)\Theta^{-1},
\]

where \( U_R(t, 0) \equiv T e^{-\int_0^t dt/H_R(t)} \). Then the state at \( t \) in the reversed process is given by

\[
\rho_R(t) = U_R(t, 0)\rho_R(0)U_R^\dagger(t, 0),
\]

Although \( \rho_f(t) \) and \( \rho_R(t) \) are far from equilibrium states, they satisfy the following lemma due to time reversal symmetry:

**Lemma.** The density matrices in the forward driving process at arbitrary time \( t \in [0, \tau] \) and its time reversed process at time \( \tau - t \) satisfy, for any finite real numbers \( a, b \in \mathbb{R} \),

\[
\text{Tr}[\Theta^{-1}\rho_f(\tau - t)\Theta^a\rho_f(t)^b] = \text{Tr}[\Theta^{-1}\rho_R(\tau)\Theta^a\rho_R(0)^b].
\]

**Proof.** From equations (18) and (19), we have

\[
\Theta^{-1}\rho_R(\tau - t)\Theta = U^\dagger_f(\tau, t)\Theta^{-1}\rho_R(0)\Theta U_f(\tau, t).
\]
Then

\[
(\Theta^{-1}\rho_R(t - \tau)\Theta)\rho_f(t),
\]

\[
= U_F^\dagger (t - \tau)(\Theta^{-1}\rho_R(0)\Theta)\rho_f(t)U_F(t, 0),
\]

\[
= U_F(t, 0)U_F^\dagger (t - \tau)(\Theta^{-1}\rho_R(0)\Theta)\rho_f(t)U_F(t, 0),
\]

\[
= U_F(t, 0)(\Theta^{-1}\rho_R(0)\Theta)\rho_f(t)U_F^\dagger (t, 0),
\]

\[
(\Theta^{-1}\rho_R(\tau - t)\Theta)\rho_f(t),
\]

which means \((\Theta^{-1}\rho_R(t - \tau)\Theta)\rho_f(t)\) and \((\Theta^{-1}\rho_R(\tau - t)\Theta)\rho_f(t)\) are related to each other by a unitary transformation \(U_F(t, 0)\). They must be equal under the trace. Thus we have proved equation \((20)\).

From the definition of quantum work distribution, we have

\[
(e^{-\beta W})^2 = Z_{eff}^{-1}\text{Tr}[U_F(t, 0)e^{-\beta(t-z)H}U_F^\dagger (t, 0)e^{-\beta H}]
\]

\[
= Z_{eff}^2\text{Tr}[U_F(t, 0)(\rho_f(t))e^{-(t-z)\rho_f(t)}U_F^\dagger (t, 0)(\Theta^{-1}\rho_R(0)\Theta)\rho_f(t)],
\]

\[
= Z_{eff}^2\text{Tr}[(\rho_f(t))e^{-(t-z)\rho_f(t)}(\Theta^{-1}\rho_R(0)\Theta)\rho_f(t)],
\]

\[
= Z_{eff}^2\text{Tr}[(\rho_f(t))e^{-(t-z)\rho_f(t)}(\Theta^{-1}\rho_R(\tau - t)\Theta)\rho_f(t)],
\]

\[
e^{-\beta \Delta F}e^{(-z-\tau)S_f[(\Theta^{-1}\rho_R(\tau - t)\Theta)\rho_f(t)]}.
\]

Here \(z\) is a finite real number and \(\Delta F \equiv F[\beta, \lambda] - F[\beta, \lambda_0]\). From equation \((29)\) to \((30)\), we have used the lemma proved above. In the last step, we have made use of definition of the order-\(z\) quantum Rényi divergence of two density matrices \(\rho_1\) and \(\rho_2\) [22, 23], \(S_z(\rho_1, \rho_2) \equiv \frac{1}{z-1}\ln\text{Tr}[\rho_1^z\rho_2^{1-z}]\), which is information theoretic generalization of standard relative entropy [19]. If we identify \(W\) - \(\Delta F\) as the dissipated work \(W_{\text{diss}}\) in equations \((26)\) and \((31)\), we therefore obtain equation \((2)\) for quantum system. Now we make several comments on equation \((2)\) for quantum system:

1) When \(z = 1\), equation \((2)\) for quantum system recovers the Jarzynski equality for quantum system.

2) The fluctuation of the dissipated work in quantum system is independent of time \(t\) because the density matrices on the right hand side of equation \((31)\) can be evaluated at any intermediate time. While the fact that it is independent of \(t\) can also be seen from \([29, 34]\). This time independence is a consequence of the time reversal symmetry.

3) For \(0 < z < 1\), the Rényi divergence for any two density matrices \(\rho_1\) and \(\rho_2\) and any quantum channel \(\varepsilon\) satisfies [20, 22]

\[
S_z[\varepsilon(\rho_1), \varepsilon(\rho_2)] \leq S_z[\rho_1, \rho_2].
\]

Therefore the quantum Rényi divergence for \(0 < z < 1\) is a valid measure of distinguishability. Thus the family of Rényi divergence appears in equation \((2)\) for quantum system is a quantification of the breaking of time reversal symmetry between the forward process and its time reversed one.

4) It relates fluctuations of the dissipated work or entropy production to the family of Rényi divergences between two non-equilibrium quantum states along the forward process and its time reversed process. Entropy production is a macroscopic quantity while the Rényi divergences between two states is essentially a microscopic quantity, which quantifies the distance between two states or to what extent the time reversal symmetry is breaking. Various moments of the dissipated work for quantum system under time-dependent driving are given by,

\[
\langle W_{\text{diss}}^n \rangle_T = T^n\text{Tr}[\rho_f(t)T_n(\ln[\rho_f(t)] - \ln[\Theta^{-1}\rho_R(\tau - t)\Theta])^n],
\]

where \(T\) is the temperature, \(n = 1, 2, 3, \cdots\) and \(T_n\) is an ordering operator which sorts that in each term of the binomial expansion of \((\ln[\rho_f(t)] - \ln[\Theta^{-1}\rho_R(\tau - t)\Theta])^n\), \(\ln[\rho_f(t)]\) always sits on the left of \(\ln[\Theta^{-1}\rho_R(\tau - t)\Theta]\). In particular for \(n = 1\), it is [29, 34, 35]

\[
\langle W_{\text{diss}} \rangle_T = TD[\rho_f(t)\ln[\rho_f(t)] - \ln[\rho_f(t)]],
\]

Here \(D[\rho_1||\rho_2] \equiv \text{Tr}[\rho_1\ln[\rho_1] - \ln[\rho_2]]\) is the von Neumann relative entropy [31, 35] between two density matrices. Recently the relation in equation \((34)\) was experimentally demonstrated by using a nuclear
magnetic resonance study of an isolated spin-1/2 system following fast quenches of an external magnetic field [36].

(5) It is an exact relation between the generating function of the dissipated work and the family of Rényi divergences between two non-equilibrium states. Thus we can extract the family of Rényi divergences from the work measurement in a driven quantum system. Since the characteristic function of quantum work distribution can be measured from the Ramsey interference of a single spin [37–39], one can also measure the family of Rényi divergences between two quantum states. We shall establish the formalism for extracting the family of Rényi divergences from Ramsey interference of a single spin in next section. Note that two recent related works connect fluctuation relations to information-theoretic concepts with more information-theoretic setting [40, 41].

4. Extracting the family of Rényi divergences from Ramsey interference of a single spin

In the recent formulation of laws in quantum thermodynamic, the family of Rényi divergences between a state and the thermal equilibrium state play a central role [42–45]. To verify the laws in quantum thermodynamics, it is also critical to measure the family of Rényi divergences. However it is quite difficult to measure the Rényi divergences from the tomographic measurement of the quantum state due to scalability problem. In section 3, we have derived the relations between dissipated work and the family of Rényi divergences. Thus we can extract the family of Rényi divergences from quantum work measurement. Work measurement in a driven quantum system is quite difficult because it requires two projective measurements of Hamiltonian [14]. However the characteristic function of quantum work distribution can be measured from Ramsey interference of a single spin [37–39]. Here we shall establish the formalism for extracting the family of Rényi divergences from Ramsey interference of a single spin. In terms of the characteristic function of the quantum work distribution, our finding, equation (2), can be written as

\[
\frac{G(i\beta \varepsilon)}{(G(i\beta))^2} = e^{e^{-1}s_{l}[p(t)\|p(t)]},
\]

(35)

Since the evaluation of the Rényi divergences is independent of time \(t\), for convenience we shall take \(t = \tau\). Thus the family of Rényi divergences can be expressed from the characteristic function of work distribution with complex arguments,

\[
S_{\varepsilon}(p(t)\|p(t)) = \frac{1}{z-1}\ln \frac{G(i\beta \varepsilon)}{(G(i\beta))^2}.
\]

(36)

The characteristic function of work distribution with real arguments can be measured from the Ramsey interference of a single spin [37–39]. To extract the family of Rényi divergences, we need to obtain the characteristic function of work distribution with complex arguments. We are now to demonstrate that the characteristic function of work distribution with complex arguments can be obtained from the characteristic function of work distribution with real arguments. This can be achieved by studying the analytic properties of the characteristic function of work distribution \(G(u)\) in the complex plane of its argument \(u\). Our results are based on the following theorems:

**Theorem 1.** For a finite quantum system with Hamiltonian \(H(\lambda)\) under a time-dependent driving process which change the Hamiltonian from a initial value \(H_i \equiv H(\lambda_i)\) to a final value \(H_f \equiv H(\lambda_f)\) in time duration \(\tau\) and is described by a unitary operation \(U(t)\), the characteristic function \(G(u)\) of the quantum work distribution is an analytic function in the complex plane of \(u\).

**Proof.** We consider the characteristic function \(G(u)\) in the complex plane of \(u\). Let us denote \(u \equiv u_R + i u_I\) and the characteristic function \(G(u) \equiv G_R(u) + i G_I(u)\). First of all, for finite quantum system we have

\[
|G(u)| = \frac{1}{Z(\beta, \lambda)}|\text{Tr}[U(\tau)e^{-i(\varepsilon + i u_I - i u_I)H_i}U^\dagger(\tau)e^{i(u_I - i u_I)H_f}]|,
\]

\[
\leq \frac{1}{Z(\beta, \lambda)}\sqrt{\text{Tr}[e^{2(i u_I - i u_I)H_f}]\text{Tr}[e^{-2i u_I H_i}]}.
\]

(37)

Here we have made use of the trace inequality \(|\text{Tr}[AB^\dagger]| \leq \sqrt{\text{Tr}[A^\dagger A]\text{Tr}[B^\dagger B]}\). Because both \(H_i\) and \(H_f\) have finite spectrum, \(G(u)\) is bounded for any finite \(u\). Second, the real part of the characteristic function is
The characteristic function $G(u)$ in the upper half complex plane, three segments at infinity in the contour integral vanish.

\[
G_R(u) = \frac{1}{2} [G(u) + G(u)^*],
\]

\[
= \frac{1}{2} \text{Tr}[U(\tau)e^{-i\beta u - i\eta t}U^\dagger(\tau)e^{i\eta t} - i\eta t H]\] + h.c.
\]

The imaginary part of the characteristic function is

\[
G_I(u) = \frac{1}{2i} [G(u) - G(u)^*],
\]

\[
= \frac{1}{2} \text{Tr}[U(\tau)e^{-i\beta u - i\eta t}U^\dagger(\tau)e^{i\eta t} - i\eta t H] - h.c.
\]

It is straightforward to prove that $G_R(u)$ and $G_I(u)$ satisfy the Cauchy–Riemann condition (appendix A), namely

\[
\partial_{\eta} G_R(u) = \partial_{\eta} G_I(u),
\]

\[
\partial_{\eta} G_R(u) = -\partial_{\eta} G_I(u).
\]

Thus we proved that $G(u)$ is an analytic function in the complex plane of $u$. The theorem 1 is proved.

**Theorem 2.** For a finite quantum system with Hamiltonian $H(\lambda)$ under a time-dependent driving process which changes the Hamiltonian from an initial value $H_0 \equiv H(\lambda_0)$ to a final value $H_f \equiv H(\lambda_f)$ in time duration $\tau$ and is described by a unitary operation $U(\tau)$, the characteristic function $G(u)$ with complex arguments are uniquely determined by the the characteristic function $G(u)$ along the real axes of $u$.

**Proof.** Define $M \equiv E_{\max}(\lambda_0) - E_g(\lambda_f)$ with $E_{\max}(\lambda)$ being the maximum eigenvalue of $H$ and $E_g(\lambda)$ being the ground state eigenvalue of $H$. According to equation (37), $|G(u)| < e^{iuM}$ as $|u| \to \infty$ in the upper half complex plane of $u$. According to theorem 1, $e^{iuM}G(u)$ is also an analytic function in the upper half complex plane of $u$ and vanishes as $|u| \to \infty$ in the upper half complex plane of $u$. Applying Cauchy integral theorem for the analytic function $e^{iuM}G(u)$, we have

\[
e^{iuM}G(u) = \frac{1}{2\pi i} \oint_C du' \frac{e^{iu'M}G(u')}{u' - u}.
\]

Here integral contour $C$ is a rectangular contour in the upper half complex plane of $u$ (figure 3). Since $e^{iuM}G(u)$ vanishes as $|u| \to \infty$ in the upper half complex plane, three segments at infinity in the contour integral vanish. Thus we have

\[
G(u) = \frac{1}{2\pi i} \int_{-\infty}^{\infty} du_R \frac{e^{i(u_R - u)M}G(u_R)}{u_R - u}.
\]

where $3u > 0$. Note that the argument of $G(u)$ on the left hand side of equation (45) is a complex number on the upper half complex plane while the argument of $G(u_R)$ on the right hand side of equation (45) is a real number. Equation (45) tells us that $G(u)$ with $3u > 0$ are determined by $G(u_R)$. Thus we proved theorem 2. Because $G(u_R)$ with real arguments can be measured by Ramsey interference of a single spin$[37–39]$, we can
Corollary 2. The free energy difference for the equilibrium states of the initial Hamiltonian $H_i$ and final Hamiltonian $H_f$ can be obtained from the characteristic function of work distribution in the non-equilibrium process which begins with the equilibrium state of the the initial Hamiltonian and ends at non-equilibrium state of final Hamiltonian

$$e^{-\beta \Delta F} = \frac{1}{2\pi i} \int_{-\infty}^{\infty} \frac{e^{i(u - u_f)G(u_f)}}{u - u_f} du_f,$$

Here $\Delta F = F(\beta, \lambda_f) - F(\beta, \lambda_i)$. Equation (48) is the exact formula for extracting the free energy difference between the equilibrium states for the initial and final control parameters from the Ramsey interference of a single spin.

According to equation (36) and theorem 2, we have

Corollary 2. The family of Rényi divergences between the the final non-equilibrium state and the equilibrium state for the final Hamiltonian can be extracted from the characteristic function of work distribution in the non-equilibrium process which begins with the equilibrium state of the initial Hamiltonian and ends at non-equilibrium state of final Hamiltonian

$$S_2[\rho_f||\rho_f(\tau)] = \frac{1}{z - 1} \ln \left( \frac{G(i\beta z)}{G(i\beta)} \right),$$

where $P(W)$ is a real function, $G(-u_R) = G(u_R)^*$. In equations (45), (48) and (49), we only need to measure $G(u_R)$ for $u_R \in [0, \infty)$. The quantum system which satisfies that $[H_i, H_f] = 0$ and $[H_i, U(\tau)] = 0$, $G(u_R)$ is a periodic function, $G(u_R + T) = G(u_R)$ and the period $T$ is determined by the energy difference of the system, then equation (45) can be simplified into

$$G(u) = \frac{1}{2i T} \int_{0}^{T} du_R \frac{e^{i(u-u_f)G(u_f)}}{\tan[(u_R - u)/T]}.$$

Equation (48) reduces to

$$e^{-\beta \Delta F} = \frac{1}{2i T} \int_{0}^{T} du_R \frac{e^{i(u-u_f)G(u_f)}}{\tan[(u_R - i\beta)/T]}.$$

Equation (49) for extracting the family of Rényi divergences becomes

$$S_2[\rho_f||\rho_f(\tau)] = \frac{1}{z - 1} \ln \left( \frac{1}{2i T} \int_{0}^{T} du_R \frac{e^{i(u-u_f)G(u_f)}}{\tan[(u_R - i\beta)/T]} \right)^2.$$
where

\[
\lambda_\tau(t) = \begin{cases} 
\lambda(t) & \text{for } 0 < t \leq \tau; \\
\lambda_\tau & \text{for } \tau < t \leq \tau + u_R, 
\end{cases}
\]  

(54)

\[
\lambda_i(t) = \begin{cases} 
\lambda_i & \text{for } 0 < t \leq u_R; \\
\lambda_i(t - u_R) & \text{for } u_R < t \leq u_R + \tau.
\end{cases}
\]  

(55)

The procedure for measuring the Ramsey inference of the probe spin is:

1. Initialize the system in the equilibrium state \( \rho_s = e^{-\beta H}/Z(\beta, \lambda_i) \) with initial Hamiltonian \( H \) and the probe spin in \( |0\rangle \) state;

2. Apply a \( \pi/2 \)-pulse along the \( y \) direction of the probe spin, which then transform the probe spin in a superposition state \( (|0\rangle + |1\rangle)/\sqrt{2} \);

3. The probe spin and the system evolve together by the Hamiltonian \( H_T \) for a time interval \( t = \tau + u_R \);

4. Apply a \( \pi/2 \)-pulse to the probe spin along the \( y \) direction;

5. Measure \( \langle \sigma_z \rangle \) and \( \langle \sigma_y \rangle \), which gives us that

\[
\langle \sigma_i(\tau + u_R) \rangle = \mathcal{R} \text{Tr}[U(\tau)e^{-iu_R H}e^{-\beta H}U^\dagger(\tau)e^{iu_R H}] / \text{Tr}[e^{-\beta H}] = \mathcal{R} G(u_R). 
\]  

(56)

\[
\langle \sigma_y(\tau + u_R) \rangle = \mathcal{I} \text{Tr}[U(\tau)e^{-iu_R H}e^{-\beta H}U^\dagger(\tau)e^{iu_R H}] / \text{Tr}[e^{-\beta H}] = \mathcal{I} G(u_R). 
\]  

(57)

Thus we can measure the characteristic function of work distribution from Ramsey interference of a single spin. To extract the free energy difference or the family of Rényi divergences we need to know \( G(u_R) \) for \( u_R \in [0, \infty) \). However in any realistic experiment we can only measure \( G(u_R) \) for a finite time duration, say \( t \in [0, T] \). Then we can use these finite time information of \( G(u_R) \) to deduce the full information of \( G(u_R) \). The reason for the validity of this method is

\[
G(u) = \int dWP(W) e^{iuW},
\]  

(58)

\[
= \sum_{m,n} \rho_m (m(\Lambda_i) |U(\tau)| n(\Lambda_i)) \chi_{m}^{\dagger} e^{i(mE_m - nE_n)},
\]  

(59)

\[
= \sum_{m,n} d_{mn} e^{i(mE_m - E_n)},
\]  

(60)

\[
= \sum_{m,n} a_{mn} \{ \cos[u(E_m^f - E_n^f)] + i \sin[u(E_m^f - E_n^f)] \}.
\]  

(61)

Thus we can make use of the following function to fit the experimental data,

\[
\tilde{G}(u) = \sum_{n=1}^{D^2} a_n \{ \cos(u\omega_n) + i \sin(u\omega_n) \},
\]  

(62)

where the number of fitting parameters is \( 2D^2 \) with \( D \) being the dimension of the system. This method was used to measure the quantum work distributions [37–39]. Note that the Jarzynski equality and the discovery in this work, equation (2), are both exact relations and in principle the equalities only hold for infinitely many trials. But in practice one can only perform finite number of trials in Jarzynski equality. Usually the convergence can be achieved with small number of trials for small system. To achieve convergence for bigger system in Jarzynski equality, more trials are required.

5. Physical model study

Here we use a specific model to verify our finding, equation (2), the relations between the generating function of work and the family of Rényi divergences.

5.1. Theoretical verification of the relation between generating function of work in non-equilibrium process and the family of Rényi divergences

Here we study an experimentally realizable system as the model example, namely, the 1D quantum transverse field Ising model. The Hamiltonian of the 1D quantum Ising model is
where $b_k, b_k^\dagger$ are the fermion annihilation and creation operators of momentum $k$, 
\[ e_k(\lambda) = 2\sqrt{1 + \lambda^2 - 2\lambda \cos k} \] is the excitation spectrum.

We now consider a sudden quench process in the 1D quantum Ising model with a transverse field. At $t = 0$, the quantum Ising model is prepared in a thermal equilibrium state with density matrix $\rho_{\text{\tiny\varepsilon}} = e^{-\beta H(\lambda)} / Z(\beta, \lambda)$. Then we suddenly change the transverse field from $\lambda_i$ to $\lambda_f$. The characteristic function of work distribution in this sudden quench process can be exactly calculated as (see appendix B for detailed derivation)
\[
G(u) = \sum_{k>0} \frac{1 + \frac{1}{2} \cos(2\alpha_k)}{\cosh(\beta e_k)},
\]
where $A_{\pm}(u) \equiv (u - i\beta) e_k^\pm \pm u e_k^- e_k^\pm$ and $e_k^\pm$ are shorthand for $e_k(\lambda)$ and $e_k(x/\lambda)$, where $\alpha_k = \theta_k - \theta_k^*$ and $\theta_k$ is defined by $\sin[2\theta_k(\lambda)] \equiv 2\sin\theta_k(\lambda)$ and $\cos[2\theta_k(\lambda)] \equiv 2(\lambda - \cos k) / e_k(\lambda)$. With this exact solution we are now ready to verify our results about the generating function of dissipated work and the family of Rényi divergences.

In the sudden quench process, the generating function of work is given by
\[
\langle \exp(-\beta W) \rangle = \frac{G(i\beta z)_{\text{\tiny\varepsilon}}}{\sum_{k>0} \frac{1 + \frac{1}{2} \cos(2\alpha_k)}{\cosh(\beta e_k)}},
\]
where we define $B_{\pm}(z) \equiv \beta(z - 1) e_k^\pm \pm \beta z e_k^- e_k^\pm$. The Jarzynski equality for free energy change is
\[
G(i\beta) = \frac{Z(\beta, \lambda_f)}{Z(\beta, \lambda_i)} = \sum_{k>0} \frac{1 + \cosh(\beta e_k)}{1 + \cosh(\beta e_k^\dagger)}.
\]
The family of Rényi divergences $S_z[\rho_i || \rho_f]$ is (see appendix B for detailed derivation)
\[
S_z[\rho_i || \rho_f] = \frac{1}{z - 1} \ln(\text{Tr}[\rho_i^z \rho_f^{1-z}]),
\]
\[
= \ln Z(\beta, \lambda_f) - \frac{e_k}{z - 1} \ln Z(\beta, \lambda_i) + \frac{1}{z - 1} \times \ln \sum_{k>0} \frac{1 + \frac{1}{2} \cos(2\alpha_k)}{\cosh(\beta e_k)}.
\]
Then it is easy to check that in the sudden quench process of the quantum Ising model, the generating function of work and the family of Rényi divergences between the initial state and the final state satisfies
\[
\langle \exp(-\beta W) \rangle = e^{-\beta \Delta F_{\text{\tiny\varepsilon}} e^{(z-1) S_z[\rho_i || \rho_f]}}.
\]
We have used a many-body system to verify that the central relation between the generating function of work distribution and the family of Rényi divergences between the final equilibrium state and the final out-of-equilibrium state.

5.2. Demonstration of measuring the family of Rényi divergences from Ramsey interference of a single spin
Here we demonstrate the scheme for experimentally measuring the family of Rényi divergences between two states, for simplicity, we consider a two spin transverse field Ising model, namely,
\[
H = -J \sigma_i^x \sigma_{i+1}^x + \lambda_i \sigma_i^z - \lambda_{i+1} \sigma_{i+1}^z.
\]
We assume that we can tune the transverse magnetic field of the first spin to be zero and then the Hamiltonian becomes
We consider $\sigma_1$ as a probe spin and $\sigma_2$ as a system. Measuring the decoherence of the first spin, which is equivalent to the characteristic function of work distribution in a sudden quench of a single spin system. The black square (circle) marks the real (imaginary) parts of the characteristic function of work distribution. The solid red line (solid blue line) is the fitting results for the real (imaginary) part of the characteristic function of work distribution.

(b) The family of Rényi divergences between the initial and final equilibrium states. The solid red line is the exact solution. The circles are obtained from the data of $G(u)$ in (a). We first using equation (62) to fit 100 evenly spaced data points of $G(u)$ shown in (a) and then making use of the fitted function to calculate the family of Rényi divergence through equation (49).

\[
H = -J\sigma_1^x \sigma_2^x - \lambda_2 \sigma_2^z.
\]

We consider $\sigma_1$ as a probe spin and $\sigma_2$ as a system. Measuring the decoherence of the first spin, which is equivalent to the characteristic function of the work distribution in a sudden quench of the second spin with the initial Hamiltonian $H_i = -\lambda_2 \sigma_2^z$ and final Hamiltonian $H_f = -\lambda_2 \sigma_2^z - J \sigma_2^x$. This is a quantum quench process and the characteristic function can be exactly evaluated to be

\[
G(u) = \frac{1}{\text{Tr}[e^{-\beta H_i}]} \text{Tr}[e^{-iuH_i}e^{-\beta H_f}e^{iuH_f}],
\]

\[
= \frac{\cosh[(\beta + iu)\lambda_2] \cos[\omega u] + i \frac{\omega}{2} \sinh[(\beta + iu)\lambda_2] \sin[\omega u]}{\cosh[\beta\lambda_2]},
\]

where $\omega \equiv \sqrt{\lambda_2^2 + J^2}$. $G(u)$ can be experimentally measured for any $u$. We shall make use of the information of $G(u)$ to extract the family of Rényi divergences between the initial equilibrium state and the final equilibrium state. We make use of $G(u)$ at inverse temperature $\beta = 1.0/\lambda_2$ and $J = \lambda_2/2$ for $u \in [0, 5/\lambda_2]$ to get the information of Rényi divergence.

In figure 4(a), we present the real (black squares) and imaginary (black circles) of the characteristic function of the work distribution in a sudden quench of a single spin from $H_i$ to $H_f$ as described above. The solid red line and solid blue line are respectively the real part and imaginary part of the characteristic function fitted by equation (62). We then make use of the fitted function to calculate the family of Rényi divergences through equation (49), which is marked by the red circles in figure 4(b). The solid red line presents the exact solution of the family of Rényi divergences. We can see that the family of Rényi divergences obtained from the characteristic function of work distributions agree well with the exact solution.
6. Conclusions

We have established an exact relation which connects a fundamental quantity in thermodynamics, the dissipated work in a system driven arbitrarily far from equilibrium, to a fundamental concept in information theory, the family of Rényi divergences. We find that the generating function of the dissipated work under an arbitrary time-dependent driving is related to the family of Rényi-divergences between the forward process and its time reversed process. Since Rényi divergences is a quantitative measure of distinguishability between two states, the Rényi divergence between the forward state and the backward state appears in equation (2) measures the breaking of time reversal symmetry. The full statistics of dissipated work in an arbitrary driving process is determined by the family of Rényi divergences. Moreover, for quantum system, one can extract the family of Rényi divergences from Ramsey interference of a single spin. In this work we studied the case that the system is isolated from the bath in the time-dependent driving process, it would be interesting to study whether the results still hold when the system and bath are coupled in the course of driven. In addition, in the recent formulation of quantum thermodynamics, the family of Rényi divergences plays a central role, it would be intriguing to find the connections of this work and the new formulation of quantum thermodynamics.

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Appendix A. Proof the real part and imaginary part of the characteristic function of quantum work distribution satisfy Cauchy–Riemann condition

In this appendix, we prove that the real part and imaginary part of the characteristic function of quantum work distribution satisfy the Cauchy–Riemann condition. The characteristic function of quantum work distribution is

\[ G(u) = \frac{\text{Tr}[U(\tau)e^{-(\beta+i\nu_k-\nu_k)H_f}U^\dagger(\tau)e^{i\nu_k-\nu_k}H_f]}{Z(\beta, \lambda)} \]  \hspace{1cm} (A1)

Its complex conjugate is given by

\[ G(u)^* = \frac{\text{Tr}[U(\tau)e^{-(\beta-i\nu_k-\nu_k)H_f}U^\dagger(\tau)e^{i\nu_k+\nu_k}H_f]}{Z(\beta, \lambda)} \]  \hspace{1cm} (A2)

The derivatives of the characteristic function with respect to the \( u_R \) and \( u_I \) respectively are given by

\[ \partial_{u_R} G(u) = -i \frac{\text{Tr}[U(\tau)H_f e^{-(\beta+i\nu_k-\nu_k)H_f}U^\dagger(\tau)e^{i\nu_k-\nu_k}H_f]}{Z(\beta, \lambda)} + i \frac{\text{Tr}[U(\tau)e^{-(\beta+i\nu_k-\nu_k)H_f}U^\dagger(\tau)H_f e^{i\nu_k-\nu_k}]}{Z(\beta, \lambda)} ] \]  \hspace{1cm} (A3)

\[ \partial_{u_I} G(u) = -i \frac{\text{Tr}[U(\tau)H_f e^{-(\beta+i\nu_k-\nu_k)H_f}U^\dagger(\tau)e^{i\nu_k-\nu_k}H_f]}{Z(\beta, \lambda)} + i \frac{\text{Tr}[U(\tau)e^{-(\beta+i\nu_k-\nu_k)H_f}U^\dagger(\tau)H_f e^{i\nu_k-\nu_k}]}{Z(\beta, \lambda)} ] \]  \hspace{1cm} (A4)

The derivatives of the complex conjugate of the characteristic function with respect to the \( u_R \) and \( u_I \) respectively are

\[ \partial_{u_R} G(u)^* = -i \frac{\text{Tr}[U(\tau)H_f e^{-(\beta-i\nu_k-\nu_k)H_f}U^\dagger(\tau)e^{i\nu_k-\nu_k}H_f]}{Z(\beta, \lambda)} - i \frac{\text{Tr}[U(\tau)e^{-(\beta-i\nu_k-\nu_k)H_f}U^\dagger(\tau)H_f e^{i\nu_k-\nu_k}]}{Z(\beta, \lambda)} ] \]  \hspace{1cm} (A5)
The real part and imaginary part of the characteristic function of work distribution is
\[
\partial_u G(u)^R = \frac{\text{Tr}[U(\tau)H_{1}e^{-(\beta-i\mu)H_{1}}U^\dagger(\tau)e^{i\mu H_{1}}]}{Z(\beta, \lambda)},
\]
\[
\partial_u G(u)^I = -\frac{\text{Tr}[U(\tau)e^{-(\beta-i\mu)H_{1}}U^\dagger(\tau)H_{1}e^{i\mu H_{1}}]}{Z(\beta, \lambda)}.
\]
(A6)

The real part and imaginary part of the characteristic function of work distribution is
\[
G_R(u) = \frac{1}{2} \left[ G(u) + G(u)^R \right],
\]
(A7)
\[
G_I(u) = \frac{1}{2i} \left[ G(u) - G(u)^R \right].
\]
(A8)

From equations (A3)–(A8), it is straightforward to check that \(G_R(u)\) and \(G_I(u)\) satisfy the Cauchy–Riemann condition,
\[
\partial_u G_R(u) = \partial_u G_I(u),
\]
(A9)
\[
\partial_u G_R(u) = -\partial_u G_I(u).
\]
(A10)

Appendix B. The characteristic function of quantum work distribution in a sudden quench of 1D transverse Ising model

In this appendix, we shall derive the characteristic function of work distribution in a sudden quench of 1D transverse Ising model. The Hamiltonian of 1D transverse Ising model with \(N\) spins is
\[
H = -\sum_{j=1}^{N}(J\sigma_j^z\sigma_{j+1}^z + \lambda\sigma_j^x),
\]
(B1)

Here periodic boundary condition is applied. The Hamiltonian is invariant under a \(\pi\) rotation along the \(z\) axis to all the spins, which is described by
\[
U_z(\pi/2) = \exp\left[i\frac{\pi}{2}\sum_j \sigma_j^z\right] = \prod_{j=1}^{N} i\sigma_j^z.
\]
(B2)

Thus the following parity operator is a conserved quantity,
\[
P = \prod_{j=1}^{N} \sigma_j^z.
\]
(B3)

It is easy to see that \(P^2 = 1\), thus parity can only take two values, \(P = \pm 1\), thus the Hamiltonian is block diagonalized,
\[
H = \begin{pmatrix} P, HP & 0 \\ 0 & P, HP \end{pmatrix} = \begin{pmatrix} H_+ & 0 \\ 0 & H_- \end{pmatrix}
\]
(B4)

where \(H_+\) is the Hamiltonian with \(P = 1\) and \(H_-\) is the Hamiltonian with \(P = -1\).

To diagonalize the Hamiltonian, we first make a Jordan–Wagner transformations, which transforms spin-1/2 to fermions,
\[
\sigma_j^z = 1 - 2c_j^\dagger c_j,
\]
\[
\sigma_j^x = \prod_{i<j} (1 - 2c_i^\dagger c_i)c_j,
\]
\[
\sigma_j^y = \prod_{i<j} (1 - 2c_i^\dagger c_i)c_j^\dagger,
\]
(B5) (B6) (B7)

where \(c_i, c_j^\dagger\) are spinless fermion operators which obey anti-commutation relations \(\{ c_i, c_j^\dagger \} = \delta_{ij}\) and \(\{ c_i, c_j \} = \{ c_i^\dagger, c_j^\dagger \} = 0\). After Jordan–Wigner transformations, the Hamiltonian is of the form,
\[
H_+ = -\sum_{j=1}^{N}(c_j^\dagger c_j) - \lambda \sum_{j=1}^{N} (1 - 2c_j^\dagger c_j),
\]
(B8)

where \(H_+\) is the fermion model transformed from spin model with even parity and it must take anti-periodic boundary condition with \(c_{N+1} = -c_1\). While \(H_-\) is the transformed free fermion model from the spin model with odd parity and it must take periodic boundary condition with \(c_{N+1} = c_1\). Note that \(H_+\) and \(H_-\) take the same form except different boundary conditions are imposed for the fermions.

The transformed fermion models are of quadratic form is a quadratic form, which can be diagonalized in the momentum space. We do Fourier transform with the prescription,
\[ c_j = \frac{1}{\sqrt{N}} \sum_k e^{i \delta_j}, \quad \text{(B9)} \]

The momentum or wave vector is fixed by the boundary condition of the fermion model: for \( H_+ \), anti-periodic boundary is imposed for fermions and the momentum is \( k_j = \frac{2 \pi j}{N} \) with \( j = -\frac{N}{2}, -\frac{N}{2} + 1, \ldots, \frac{N}{2} - 1 \) if \( N \) is even and \( j = -\frac{N-1}{2}, \ldots, \frac{N-1}{2} \) if \( N \) is odd. For \( H_- \), the fermion model should take periodic boundary condition and the momentum is given by \( k_j = \frac{2 \pi j}{N} \) with \( j = -\frac{N}{2}, -\frac{N}{2} + 1, \ldots, \frac{N}{2} - 1 \) if \( N \) is even and \( j = -\frac{N-1}{2}, \ldots, \frac{N-1}{2} \) if \( N \) is odd. After the Fourier transformation, we have

\[ H_k = \sum_k \left( 2 \lambda - 2f \cos k \right) \left( c_j^+ c_k - \frac{1}{2} \right) - i e^{i k} c_j^+ c_{-k} + i e^{-i k} c_k c_{-j}. \quad \text{(B10)} \]

Since \( k \) and \( -k \) are coupled, it is instructive to write the Hamiltonian in the following form

\[ H_{k \pm} = \sum_{k > 0} \left[ E_k (c_j^k c_k + c_j^c_{-k} - 1) - i \Delta_k (c_j^c_{-k} c_k + c_k c_{-j}) \right], \quad \text{where} \quad H_k = E_k - i \Delta_k \begin{pmatrix} 0 & 0 & i & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \quad \text{(B11)} \]

The momentum or wave vector is \( k_j \) and the momentum is given by \( k_j = \frac{2 \pi j}{N} \) with \( j = -\frac{N}{2}, -\frac{N}{2} + 1, \ldots, \frac{N}{2} - 1 \) if \( N \) is even and \( j = -\frac{N-1}{2}, \ldots, \frac{N-1}{2} \) if \( N \) is odd. After the Fourier transformation, we have

\[ H_k = \left( \begin{array}{cccc} E_k - i \Delta_k & 0 & 0 & 0 \\ 0 & -E_k & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{array} \right) \equiv h_k + O_{2 \times 2}. \quad \text{(B12)} \]

Defining \( \tau^\prime_k \), the pauli matrices in the subspace of two stats of momentum \( k \), namely \( | \uparrow \rangle = | E_k, 1_{-k} \rangle \) and \( | \downarrow \rangle = | 0_k, 0_{-k} \rangle \),

\[ h_k = E_k \tau^\prime_k + \Delta_k \tau^\prime_k, \quad \text{(B14)} \]

where we define \( E_k = \sqrt{E_k^2 + \Delta_k^2} \) and \( \cos \theta_k = \frac{E_k}{\sqrt{E_k^2 + \Delta_k^2}} \) and \( \sin \theta_k = \sqrt{1 - \cos^2 \theta_k} \).

Because

\[ e^{i \theta_k \gamma_5 / 2} = \cos \frac{\theta_k}{2} + i \sin \frac{\theta_k}{2} = \begin{pmatrix} \cos \frac{\theta_k}{2} & i \sin \frac{\theta_k}{2} \\ i \sin \frac{\theta_k}{2} & \cos \frac{\theta_k}{2} \end{pmatrix}, \quad \text{(B18)} \]

the Hamiltonian can be written in matrix form in the subspace of \( | \uparrow \rangle = | E_k, 1_{-k} \rangle \) and \( | \downarrow \rangle = | 0_k, 0_{-k} \rangle \) as

\[ h_k = \begin{pmatrix} \cos \frac{\theta_k}{2} & i \sin \frac{\theta_k}{2} \\ i \sin \frac{\theta_k}{2} & \cos \frac{\theta_k}{2} \end{pmatrix} \begin{pmatrix} E_k & 0 \\ 0 & -E_k \end{pmatrix} \begin{pmatrix} \cos \frac{\theta_k}{2} & i \sin \frac{\theta_k}{2} \\ i \sin \frac{\theta_k}{2} & \cos \frac{\theta_k}{2} \end{pmatrix}. \quad \text{(B19)} \]

Note that each matrix elements in \( h_k \) are functions of the parameter of the system, \( f \) and \( \lambda \). The partition function of transverse Ising model at inverse temperature \( \beta \) is

\[ Z(\beta, \lambda) = \text{Tr}[e^{-\beta H} \prod_{k > 0} e^{-\beta h_k}], \quad \text{where} \quad \lambda = \exp(-\beta \Delta), \quad f = \exp(-\beta \Delta) \]

\[ = \prod_{k > 0} \text{Tr}[e^{-\beta \Delta}], \quad \text{(B21)} \]

\[ = \prod_{k > 0} [e^{-\beta \Delta} + e^{\beta \Delta} + 1], \quad \text{(B22)} \]

\[ = \prod_{k > 0} 2 \cos(\beta \Delta) + 1. \quad \text{(B23)} \]
where \( \epsilon_k \equiv \epsilon_k(\lambda) \). To calculate the characteristic function of work distribution, we first evaluate

\[
U_k[\tau, \lambda] \equiv \exp\{-itH_k(\lambda)\} = e^{it\theta_k} \exp\{i \Omega_{2,2}\} = e^{it\theta_k} \oplus I_2 \times 2_2,
\]

\[
= \left( \begin{array}{cc}
\cos \frac{\theta_k}{2} & i \sin \frac{\theta_k}{2} \\
- i \sin \frac{\theta_k}{2} & \cos \frac{\theta_k}{2}
\end{array} \right) \left( \begin{array}{cc}
e^{-i\epsilon_k(\lambda)} & 0 \\
0 & e^{i\epsilon_k(\lambda)}\end{array} \right) \left( \begin{array}{cc}
\cos \frac{\theta_k}{2} & - i \sin \frac{\theta_k}{2} \\
- i \sin \frac{\theta_k}{2} & \cos \frac{\theta_k}{2}
\end{array} \right) \oplus I_2 \times 2_2.
\]

\[
= \left( \begin{array}{cc}
\cos (\epsilon_k(\lambda)) - i \sin (\epsilon_k(\lambda)) \cos \theta_k & - \sin (\epsilon_k(\lambda)) \sin \theta_k \\
\sin (\epsilon_k(\lambda)) \sin \theta_k & \cos (\epsilon_k(\lambda)) + i \sin (\epsilon_k(\lambda)) \cos \theta_k
\end{array} \right) \oplus I_2 \times 2_2.
\]

(B24)

Note that \( \epsilon_k \) and \( \theta_k \) are functions of the parameters of the Hamiltonian.

Now we are ready to calculate characteristic function of quantum work distribution in a sudden quench of the transverse Ising model from \( H_I \) to \( H_F \), which is defined by

\[
G(u) = \frac{1}{Z(\beta, \lambda_k)} \det \left[ e^{-\beta H_I} e^{-\beta \epsilon u} e^{i\epsilon u} \right],
\]

(B25)

\[
= \frac{1}{Z(\beta, \lambda_k)} \det \left[ e^{-\beta H_I} e^{i\epsilon u} \right],
\]

(B26)

\[
= \frac{1}{Z(\beta, \lambda_k)} \prod_{k=0}^N \det \left[ e^{-\beta H_I} e^{i\epsilon u} \right],
\]

(B27)

\[
= \frac{1}{Z(\beta, \lambda_k)} \prod_{k=0}^N \det \left[ T_k(u - i\beta) U_k(-u, \lambda_k) \right],
\]

(B28)

\[
= \prod_{k=0}^N \left[ 1 + \frac{1 + \cos(\alpha_k) + \cos(\epsilon_k)}{2} \right] \cos[A_1(u)] + \frac{1 - \cos(\alpha_k) - \cos(\epsilon_k)}{2} \cos[A_2(u)].
\]

(B29)

where we define \( \alpha_k = \theta_k - \theta_k, A_1(u) \equiv (u - i\beta)^1 + u\epsilon_k \) and \( A_2(u) \equiv (u - i\beta)^1 - u\epsilon_k \).

The momentum \( k = \frac{2i\lambda - 1}{N}, \ j = \ 1, 2, 3, \cdots, \left[ \frac{N}{2} \right] \).

The family of Rényi divergences between the equilibrium states for the initial and final parameters \( \rho_1 \) and \( \rho_2 \), are

\[
S_\lambda[\rho_1||\rho_2] = \frac{1}{z - 1} \ln(\det[\rho_2^{1/z} \rho_1^{1/z}]),
\]

\[
= \ln Z(\beta, \lambda) - \frac{z}{z - 1} \ln Z(\beta, \lambda) + \frac{1}{z - 1} \ln \det[\exp[-\beta(1 - z) H] e^{-\beta \epsilon}],
\]

(B30)

\[
= \ln Z(\beta, \lambda) - \frac{z}{z - 1} \ln Z(\beta, \lambda) + \frac{1}{z - 1} \ln \det[\exp[-\beta(1 - z) H] e^{-\beta \epsilon}],
\]

(B31)

\[
= \ln Z(\beta, \lambda) - \frac{z}{z - 1} \ln Z(\beta, \lambda)
\]

(B32)

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