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Quantum Irreversibility in a Misaligned Spin System

Selçuk ÇAKMAK*[1]

Abstract

A single spin that is misaligned with respect to the static external magnetic field is investigated as a toy model to clarify the nature of irreversibility in terms of inner friction and irreversible work. The coherence generation and the effects of unwanted transitions are analyzed in detail. The behavior of inner friction and irreversible work as a function of protocol time are analyzed for a finite-time unitary transformation. The coherence generation is shown to be the common sign for the inner friction and irreversible work. The excess energy sourced by the unwanted transitions for a quasistatic transformation is found to be the only sign for irreversible work. The angle dependencies of the inner friction and irreversible work are also analyzed explicitly. The selected model and the considered realistic parameters are available to be implemented for the finite-time operations on the nuclear magnetic resonance setups.

Keywords: Quantum thermodynamics, Nonequilibrium and irreversible thermodynamics, Irreversible work, Inner friction

1. INTRODUCTION

The fast driving protocols are required for powerful thermal heat engines and refrigerators which are, however, the source of irreversibility [1-21]. In the scales where the quantum fluctuations are also relevant, the two irreversibility measures named recently as the inner friction and irreversible work have been introduced as two distinct irreversibility quantifiers that arise from the fast Hamiltonian driving protocols [14,16]. The inner friction and the irreversible work can be considered as the system response to the external driving techniques. The mechanism of the system response can be explained fully with the quantum mechanical theory. The initial studies on the concept of inner friction and irreversible work are realized on various models [12-19]. The inner friction has been recently investigated in ref [14] considering misalignment and disordered samples. There have been studies that investigate the effects of inner friction on work output and the efficiency of the quantum counterpart of classical Otto and Carnot heat engines [16,19]. The finite-time driven quantum two-level system undergoing the unitary evolution shows that the quantum friction arises in the case of the fast-driven model. The basic reason is explained according to the quantum adiabatic theorem as the system cannot follow its instantaneous eigenstates

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[12,16,17]. On the other hand, the irreversible work and inner friction are investigated analytically considering reversible isothermal and reversible adiabatic conditions [12].

The inner friction or irreversible work can be defined from the comparison of the work done on the system during the actual finite time process with the one obtained along the ideal adiabatic or isothermal process (see Figure 1). The quantum relative entropy, which is one of the basic distance measurement between two quantum states, has been recently connected both to the inner friction and the irreversible work [12]. The connection shows here that the measures treated an equal footing. The reasons for arising entropy in terms of quantum relative entropy during finite-time unitary driving are investigated in detail in ref [18]. The population mismatch and the coherence generation are reported as two basic contributions to entropy production [18].

In this study, we focus on the finite-time unitary-driven of a spin-$1/2$ system that is misaligned with respect to the external static magnetic field. We analyze the energetic deviation from the reversible quantum adiabatic and reversible quantum isothermal transformation under realistic conditions. The role of misalignment and the total protocol time on the inner friction and the irreversible work are investigated in detail. Also, the coherence and the population mismatch effects on the inner friction and irreversible work are explicitly revealed. The obtained results indicate the differences between the inner friction and irreversible work inevitably arises from the population mismatch contribution.

2. THEORY

2.1. Irreversible Work

A thermal equilibrium state with inverse temperature β_i $(1/k_B T_i)$ is defined by Boltzmann-Gibbs distribution [15]. Unitary driving leads to the initial system represented by ρ_0 to out of the equilibrium state, $\rho_0 \rightarrow \rho_\tau$, which causes the energetic deviation from the reversible state (isothermal transformation) which is driven quasi-statically isothermal $(\beta_i = \beta_B)$, $\rho_0 \rightarrow \rho_B$. This energetic deviation indicates dissipated work from the system, known as irreversible work. More precisely, the irreversible work is the difference between the work obtained through unitary transformation and the one through the reversible isothermal process (see Figure 1). The magnitude of the energetic deviation from the reversible state is related to the quantum relative entropy, $D(\rho_\tau||\rho_B) = tr[\rho_\tau(\ln\rho_\tau - \ln\rho_B)]$. Thus, the irreversible work can be given as [12]

$$\langle\omega_{irr}\rangle = \beta^{-1}[D(\rho_\tau||\rho_B)]. \quad (1)$$

The unitary driving protocol is followed by a relaxation process in which the system reaches a thermal equilibrium state via dissipate energy into the heat bath, evolves naturally.

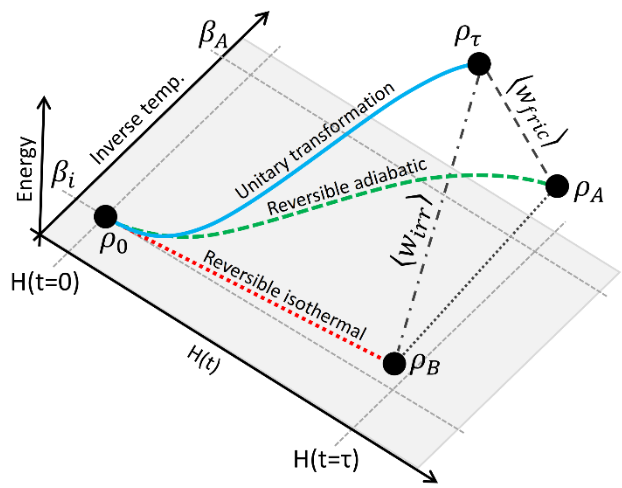

Figure 1 Sketch of the transformations discussed in the text. All the transformations are considered to start with an initial thermal state at inverse temperature β_i. The blue solid line indicates parametric finite time (unitary) transformation of the system Hamiltonian from $H(t=0)$ to $H(t=\tau)$ in a time interval τ. The state ρ_τ defined at the end of the unitary process is a nonequilibrium state due to the inter-level transitions. The green dashed and red dotted lines are the reversible adiabatic and isothermal processes which define effective thermal states corresponding to $H(t=\tau)$ as denoted by ρ_A and ρ_B, respectively. The relative entropy of ρ_τ to ρ_A or to ρ_B gives the inner friction or irreversible work as indicated by black dashed and dash-dotted lines, respectively.

The Eq. 1 enables the exploration of the different contributions on the irreversible work by the separation approach in Ref. [18]. The population mismatch measured by the difference in populations between ρ_τ and ρ_B, which is caused by unwanted transitions and the coherence generated in the unitary driving operation are two quantitative contributions to irreversible work. The coherence generated in the process can be defined as [18]

$$C(\rho_\tau) = D(\rho_\tau||\Delta[\rho_\tau]) = S(\Delta[\rho_\tau]) - S(\rho_\tau) \quad (2)$$

Where $\Delta[\rho_\tau]$ is the density matrix in the energy basis of system at the end of unitary driving. $S(\Delta[\rho_\tau])$ and $S(\rho_\tau)$ are von Neumann entropy $\left(S(\rho) = -tr(\rho \ln \rho)\right)$. Considering Eq. 2 the irreversible work can be reformed as [18]

$$\langle \omega_{irr} \rangle = \frac{1}{\beta_i}[C(\rho_\tau) + D(\Delta_\tau[\rho_\tau]||\rho_B)]. \quad (3)$$

This equation explains that the finite-time transformations can generate coherence and make an unstable distribution of the populations with respect to ρ_B. These are two measurable indicators for the irreversible work, quantitatively.

2.2. Inner Friction

The difference between the work performed on the system during the actual unitary process and the reversible adiabatic one, however, defines the inner friction (see Figure 1). The reversible adiabatic transformation requires the protection of the population of each energy level. This is possible with infinite time unitary driving ($\tau \to \infty$). At the end of the reversible adiabatic transformation, the system reaches to desired state, ρ_A. Also, the system can follow its instantaneous eigenstates. The reversible adiabatic state, $\rho_A = \sum_n P_n^{(0)} \left|\epsilon_n^{(A)}\right\rangle\left\langle\epsilon_n^{(A)}\right|$ where the $P_n^{(0)}$ is initial population of n^{th} energy level and $\left|\epsilon_n^{(A)}\right\rangle$ is the eigenstate of the H_A. On the other hand, the fast-driving protocols, generally, cause the deviation from the desired state which is obtained by the reversible adiabatic transformation, ρ_A. So, this deviation requires extra work on the system to reach the desired state, ρ_A. The extra work mentioned here is called inner friction. The amount of extra work depend the duration of finite-time transformation, τ. The distance between the desired state and the reached state via finite time driving is a quantitative measurable indicator. The quantum relative entropy is a useful tool to measure the amount of the distance between ρ_τ and ρ_A, $D(\rho_\tau||\rho_A)$. Besides, the system releases the excess energy-sourced by the finite-time transformation, as heat form to the heat bath. The inverse temperature of the heat bath is β_A $(1/k_B T_A)$. Thus the inner friction is defined as below [12]

$$\langle \omega_{fric} \rangle = \beta^{-1}[D(\rho_\tau||\rho_A)] \geq 0. \quad (4)$$

Since the inner friction can be given by the quantum relative entropy a similar contribution separation as given in Eq. 3 can also be done for the inner friction.

3. RESULTS

The considered system Hamiltonian of a two-level single spin interacting to the time-dependent magnetic field along the z-axis and x-axis, could be defined as [14]

$$H(t) = \Omega_0 I_z + \Omega(t)(\cos\theta\, I_z + \sin\theta\, I_x). \quad (5)$$

Where Ω_0 is the static magnetic field along the z-axis, the $\Omega(t)$ is externally controlled time-dependent magnetic field and θ is the misaligned angle of spin with respect to the static magnetic field.

During the finite time transformation, we tune the magnetic field from its initial Ω_i to a final Ω_f value. It changes linearly with time t. The driving function is given as

$$\Omega(t) = \Omega_i\left(1 - \frac{t}{\tau}\right) + \Omega_f\left(\frac{t}{\tau}\right), \quad (6)$$

where $\Omega_f = 2\Omega_i$ and $\Omega_i = \Omega_0$. The τ is the duration of the finite-time transformation. Also, the finiti-time transformation can be described by a unitary evolution of the density matrix expressed by von Neumann equation $\dot{\rho}(t) = -i[H(t), \rho(t)]$. The density matrices of the initial and final states are ρ_0 (where $t = 0$) and ρ_τ (where $t = \tau$), respectively.

For the above discussed driving protocol (Eq. 6), on the considered model (Eq. 5), we now investigate the role of the misalignment and the total time allocated to the protocol on the irreversible work and inner friction given by Eqs. 1 and 4, respectively. To see the possible existence of the irreversibility in a quantum system that can be experimentally achievable, we chose the parameters which are thermodynamically implemented in liquid state nuclear magnetic resonance (NMR), recently [19]. Therefore, we set the bath temperature at $T = 10\ peV/k_B$ and the frequency at $\Omega_0 = 2\pi f$ here $f = 2\ kHz$ with considering the misalignment angles as $\left\{0, \frac{\pi}{5}, \frac{\pi}{4}, \frac{\pi}{3}, \frac{\pi}{2}\right\}$.

We first investigate the inner friction given the Eq. 4 and plot the inner friction versus the total protocol time for different misalignment angles. Please recall here that the density matrix for the reversible adiabatic may be written in the form as $\rho_A = \sum_n P_n^{(0)} \left|\epsilon_n^{(A)}\right\rangle\left\langle\epsilon_n^{(A)}\right|$ which is constructed in terms of initial level populations $P_n^{(0)}$ and the final eigenstates of the Hamiltonian $H(t=\tau)$. The state ρ_A for a qubit is infected an effective thermal state at temperature τ_A, i.e, $\rho_A = e^{-\beta_A H(t=\tau)}/Z_A$, where $Z_A = tr\left[e^{-\beta_A H(t=\tau)}\right]$. The inner friction quantifies how the density matrix defined at the end of the parametric finite-time transformation deviates from the reversible correspondence ρ_A. Figure 2 shows that we obtain zero inner friction at the quasi-static regime $(\tau = 0)$ and without misalignment $(\theta = 0)$. The former is the consequence of the celebrated quantum adiabatic theorem in which the system density matrix follows the instantaneous eigenstates without changing the initial level populations. The latter one is due to the absence of time-ordering in the unitary time evolution in the case of $[H(t = t_1), H(t = t_2)] = 0$ which results also zero inner friction. On the other hand, when the Hamiltonian at different time instants is incompatible, (when $0 < \theta \leq \pi/2$) we obtain non-zero inner friction for a finite-time transformation as shown in Figure 2. The inner friction is high for a fast-transformation (small τ values) which decays almost exponentially as a function of τ. The transformation considered here can be regarded as fast or slow by making interpretation using the energy-time uncertainty relation [22]. If we denote ΔE as the minimum energy gap between the energy levels during the transformation, then one can name the transformation, physically, as fast when $\tau \ll \hbar/\Delta E$ or slow when $\tau \gg \hbar/\Delta E$ [23]. For a given τ, we obtain higher inner friction for a larger misalignment θ since the angle, θ, affects the eigenenergies and leads to higher system energies for a larger θ.

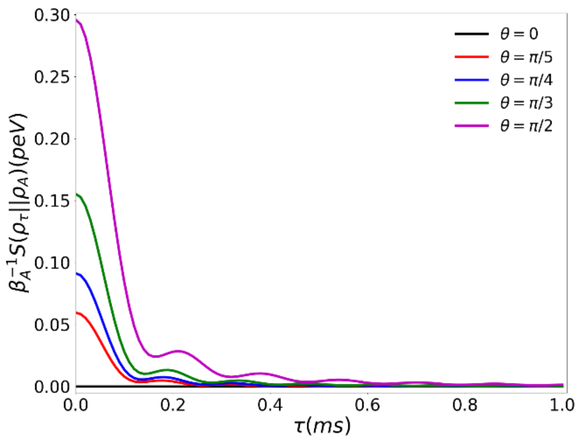

Figure 2 Inner friction arises in unitary transformation as a function of driving time τ for different misalignments θ, at $T_i = 10\ peV/k_B$.

The second considered irreversibility measure is the irreversible work which is defined as the relative entropy of ρ_τ to the state at the end of the reversible isothermal processes, ρ_B. Figure 3 shows the irreversible work as a function of protocol time for different misalignment angles θ. The irreversible work is always non-zero even in the case of zero misalignment $\theta = 0$ and in the quasi-static regime $(\tau \to \infty)$ due to the population mismatch between the final states ρ_τ and ρ_B (which will be discussed later in the text in detail). For non-zero misalignment $(0 < \theta \leq \pi/2)$, we obtain higher irreversible work for the fast transformation which decays to a non-zero stable value as τ increases. In contrast to inner friction as shown in Figure 2, the irreversible work is always greater than zero and approaches to larger non-zero stable values for larger misalignment not only at quasistatic regime but also at a finite-time transformation. This effect is originated from the population mismatch between the states ρ_τ and ρ_B as we will discuss as a next.

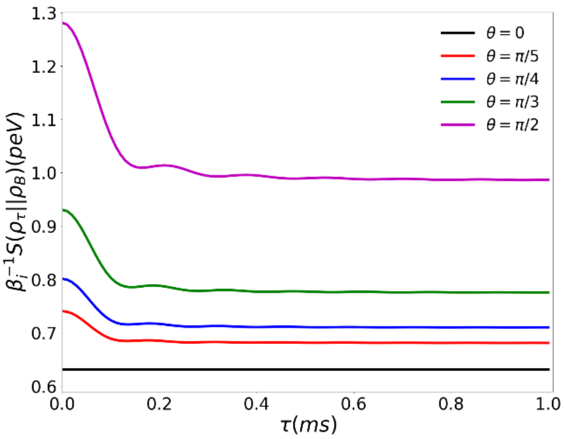

Figure 3 The irreversible work dissipated from the system as a function of the driving time τ for different misalignments θ, at $T_i = 10\ peV/k_B$.

We now investigate the mechanisms that contribute to inner friction and irreversible work. According to Eq. 3, there are two contributions to irreversibility. The first is coming from the coherence generation in τ_A during the finite time parametric transformation and the other one is the population mismatch between the state ρ_τ and the target states defined at the end of reversible transformations (i.e., ρ_A and ρ_B). In Figure 4 (a), we present the contributions on the irreversibility using Eq. 3 as a function of protocol time for the misalignment $\theta = \pi/4$. The coherence generation contribution is shown in Figure 4 (b) is the same for both the inner friction and the irreversible work since $C(\rho_\tau)$ measures the coherence generation in the energy frame during the finite time process. For a fast process, the coherence generation is high which decays and becomes zero at the quasistatic limit as predicted by the quantum adiabatic theorem.

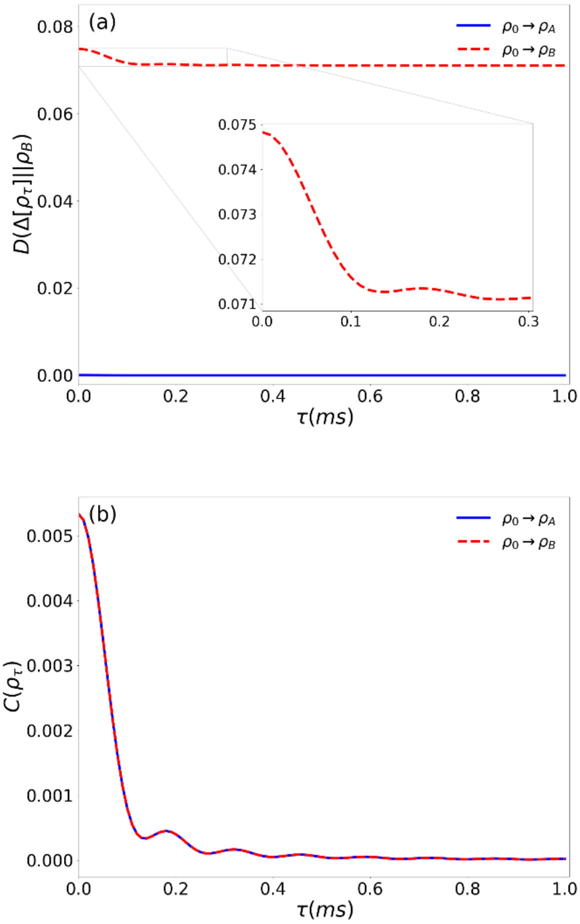

Figure 4 Population mismatch (a) and coherence generation (b) contributions to the irreversible work (dashed-red) and inner friction (solid-blue) as a function of driving time τ. The inset in (a) shows a magnification to the population mismatch effect for irreversible work.

The difference between the inner friction and irreversible work comes from the population mismatch contribution. For a fast transformation, the population mismatch is high for both cases. Since the final state ρ_τ approaches to ρ_A in the quasistatic limit, the population mismatch contribution on the inner friction decays to zero as τ increases. For the irreversible work case, the population mismatch contribution, however, approaches to a non-zero stable value as τ increases. Therefore, we conclude here that this is the population mismatch contribution that leads to differences between the two irreversibility measures and the non-zero stable value for the irreversible work at the quasistatic transformation limit.

4. CONCLUSIONS

We have investigated the concepts of irreversible work and inner friction for a driven single spin misaligned with respect to the external static magnetic field. The relative entropy between the actual state obtained at the end of the parametric finite-time transformation and the state obtained in a reversible adiabatic or a reversible isothermal transformation is a quantitative measure for the inner friction or irreversible work. The irreversibility measures are analyzed as a function of protocol time at different misalignment angles for the eligible parameters for NMR setups. For a finite-time transformation, we found a large deviation from the target states indicating the irreversibility in our setting. The mechanisms that contribute to the irreversibility measures have been also investigated. We emphasize that the coherence generation is the same for both inner friction and irreversible work. The differences between the irreversible work and the inner friction are found to be originated from the population mismatch contribution between the target states and the one obtained at the end of the unitary protocol.

We would like to remark here that the typical energy gaps and the heat source energy $k_B T_i$ a few peVs. Therefore, the irreversible work and the inner friction shown in Figures 2 and 3 are on the same order of magnitude which is also a few peVs for the finite-time transformation. For the considered operation regime, both thermal and quantum fluctuations affect the protocol adopted here. Here we elucidate how the quantum fluctuations associated with the coherence generation in the energy frame due to the fast driving leads to irreversibility from two different perspectives of definitions.

In NMR, the characteristic decoherence times are in order of seconds. On the other hand, the time allocated to the considered unitary driving protocol is in order of milliseconds. We, therefore, conclude here that the results obtained for the irreversible work and friction can be realized by using the NMR techniques [10, 24, 25].

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The Declaration of Conflict of Interest/ Common Interest

No conflict of interest or common interest has been declared by the author.

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