
# Improve The Convergence of Jarzynski Equality through Fast-Forward Adiabatic Process: Quantum Systems

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April 2014

# *Abstract*

The discovery of Jarzynski Equality relates the work statistics during a non-equilibrium process to the equilibrium free energy difference. Its application is, however, greatly limited by the poor convergence. We adopt the method of fast-forward adiabatic driving which is firstly raised by S. A Rice to improve the convergence. We follow Berry's approach of transitionless quantum driving and study on the convergence of quantum systems by comparing the convergence of Jarzynski equality under non-adiabatic and fast-forward adiabatic process. We illustrate our method on a two-level system and 1-D harmonic oscillator at different temperatures and discuss how temperature and negative work due to transitions between instantaneous eigenstates affect the convergence. We also study the relation between the degree of adiabaticity of a process and the convergence of Jarzynski equality.

# *Acknowledgements*

I gratefully acknowledge the useful discussion with Gaoyang Xiao and help from Hailong Wang and my supervisor Prof Jiangbin Gong.

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# Chapter 1

# Introduction

Since the discovery of fluctuation theorems [1] which are also known as Jarzynski equality [2] and Crooks relation [3], lots of attention has been paid to the field of nonequilibrium statistical mechanics and thermodynamics. They characterize and restrict the form of work function for a driven system initialized in thermal equilibrium. When first discovered, the relations were formulated for closed classical system. Researcher subsequently generalized them to open classical systems [4], quantum systems [5] and systems where generalized measurements interrupt the force protocol [6, 7]. Experimentalists also tested the validity of these relations in the laboratory in both classical regime and quantum regime [8–10].

The discovery of Jarzynski equality signifies that people have a much deeper understanding on nonequilibrium statistical mechanics and thermodynamics. Its application is, however, often limited by its poor convergence. To resolve the problem, physicists have made a lot of efforts [11, 12] and have made significant progress. Reference [11] pointed out the importance of dissipated work which is defined as the difference between expected work and Helmholtz free energy difference and suggested that a reduction in the dissipated work would greatly improve the convergence.

The nature of Jarzynski convergence is simply the expectation of a probability distribution of one exponential form of work. From our knowledge of statistics, some factors which might affect the convergence would be variance and the existence of extreme values. A smaller variance, in other words, a more concentrated probability distribution is expected to lead to a faster convergence. Also, when there exist extreme values, the convergence is likely to be delayed. With a more

concentrated work distribution for adiabatic process [13], we hope that adiabatic process would produce a better result. As the conventional adiabatic process takes a long time to accomplish, based on recent work on transitionless quantum driving [14], we accelerate the adiabatic process by adding a control Hamiltonian to the original Hamiltonian. We study the convergence of Jarzynski equality under this fast-forward adiabatic process and a normal non-adiabatic process to see how the method of fast-forward adiabatic process improves the convergence. Meanwhile, we discuss the importance of temperature and negative work due to transitions between instantaneous eigenstates (In the rest of the report, "work due to transitions between instantaneous eigenstates" is simply referred as "negative work" for convenience.) during the convergence by comparing the rate of convergence under different temperatures and analysing the negative-work realizations. We also study the relation between the degree of adiabaticity of a process and the convergence of Jarzynski equality. The essential objective of this project is to enhance the fundamental understanding of Jarzynski equality and improve its convergence by suppressing work fluctuations with fast-forward adiabatic process.

The rest of this report is arranged in the following manner. We will first review Jarzynski's equality in the second chapter, followed by the quantum adiabatic theorem and transitionless quantum driving in the third chapter. After that, we will show our study on the improvement of the convergence of Jarzynski equality with the adoption of fast-forward adiabatic process. In this part, we study on a two-level system and 1-D quantum harmonic oscillator. The convergence under non-adiabatic and fast-forward adiabatic process is studied and the effect of temperature and negative work is discussed and the relation between the degree of adiabaticity and the convergence of Jarzynski equality is obtained. The report is ended with a short conclusion.

# Chapter 2

# Jarzynski Equality

Jarzynski equality was first discovered in 1997 by Christopher Jarzynski [2]. It is described by the equation $\langle e^{-\beta W} \rangle = e^{-\Delta F}$. The equation says the expected exponential of work done to a system during a force protocol equals the exponential of Helmholtz free energy difference between two equilibrium thermal states. This is a very significant and powerful property as it relates the non-equilibrium quantity $W$ with the equilibrium quantity $\Delta F$. Theoretically, it suggests a deeper understanding of non-equilibrium statistical mechanics and thermodynamics. Practically, it could be applied in the free energy estimation and this is of great importance in biomolecular system studies where the free energy difference is a vital property, for instance, the measurement of free energy increase of a protein when its length is changed.

In this chapter, we will review the original Jarzynski equality in classical systems and its quantum version. Particularly, we will give a detailed work of how Jarzynski equality is derived in quantum systems.

## 2.1 Jarzynski Equality in classical system

The Jarzynski equality relates work statistics with the Helmholtz free energy difference. The first thing to make clear is the definition of work in the classical system considered. Here we follow the approach of inclusive work [15] and consider a classical system which is not in contact with the heat reservoir. Thus, the

work is given by the energy difference between the initial and final state of the system.

We look at a system described by the Hamiltonian $H(\lambda(t), \mathbf{z}(t))$ and evolving from time 0 to $\tau$, where

$$\mathbf{z}(t) = [\boldsymbol{p}(t), \boldsymbol{q}(t)] \tag{2.1}$$

represents the evolution trajectory of the system and $\lambda(t)$ is a time dependent parameter specifying the time dependence of the Hamiltonian. During the process, the work W done to the system could be given by

$$W_\tau = H(\lambda(\tau), \mathbf{z}(\tau)) - H(\lambda(0), \mathbf{z}(0)). \tag{2.2}$$

To review the Jarzynski equality in classical system, we consider a Gibbs canonical ensemble and assume the initial state of the system is in equilibrium. With $(\lambda(0), \mathbf{z}(0)$ being the initial condition, the probability distribution at time 0 would be

$$\rho(\lambda(0), \mathbf{z}(0)) = \frac{e^{-\beta H(\lambda(0), \mathbf{z}(0))}}{Z_0}, \tag{2.3}$$

where

$$Z_t = \int_\Gamma e^{-\beta H(\lambda(t), \mathbf{z}(t))} d\mathbf{z}(t), \tag{2.4}$$

is the partition function of the system at time $t$. The expected exponential of work done to the system during the process is then

$$\begin{aligned} \langle e^{-\beta W} \rangle &= \int_\Gamma \rho(\lambda(0), \mathbf{z}(0)) e^{-\beta W_\tau} d\mathbf{z}(0) \\ &= \int_\Gamma \frac{e^{-\beta H(\lambda(0), \mathbf{z}(0))}}{Z_0} e^{-\beta [H(\lambda(\tau), \mathbf{z}(\mathbf{z}(0), \tau)) - H(\lambda(0), \mathbf{z}(0))]} d\mathbf{z}(0) \\ &= \frac{Z_\tau}{Z_0}. \end{aligned} \tag{2.5}$$

In the last step, we have performed a canonical transformation $\mathbf{z}(0) \to \mathbf{z}(\mathbf{z}(0), \tau)$ where the Jacobian is 1. The Helmholtz free energy expressed by partition function is $F = -\frac{1}{\beta} \ln Z$. Plugging this expression into equation (2.5), we obtained the Jarzynski equality in classical system:

$$\langle e^{-\beta W} \rangle = \frac{e^{-\beta F_\tau}}{e^{-\beta F_0}} = e^{-\beta \Delta F}. \tag{2.6}$$

Soon after the discovery of Jarzynski equality in classical systems, the validity of the equation is verified in quantum systems theoretically.

## 2.2 Jarzynski equality in quantum system

In quantum systems, the work would be a bit different. One general definition of work which is based on the two-time projective energy measurement is $W_{mn} = E_m^\tau - E_n^0$. $E_n^0$ is the eigenenergy of the system when the initial state is $|n_{\lambda(0)}\rangle$ and $E_m^\tau$ is eigenenergy of the system at time $\tau$ when the final state is $|m_{\lambda(\tau)}\rangle$ with $|n_{\lambda(t)}\rangle$ being the instantaneous eigenstate of the system which is described by the Hamiltonian $\hat{H}_0(\lambda(t))$. Again, the time-dependent parameter $\lambda(t)$ specifies the time dependence of the Hamiltonian. The major difference between classical and quantum systems when we derive Jarzynski equality is that in quantum systems, $e^{-\beta\hat{H}_0(\lambda(0))}$ does not annihilate with the $\beta\hat{H}_0(\lambda(0))$ part in $e^{-\beta(\hat{H}_0(\lambda(\tau))-\hat{H}_0(\lambda(0)))}$ because they do not commute for a time-dependent Hamiltonian $\hat{H}_0(\lambda(t))$.

To see the quantum Jarzynski equality, we consider a quantum system which is in thermal contact with a heat bath with inverse temperature $\beta$ before time 0 so that the system is prepared in the equilibrium thermal state:

$$\rho(0) = Z_0^{-1} \exp\{-\beta\hat{H}_0(\lambda(0))\}, \tag{2.7}$$

with $Z_0 = Tr \exp\{-\beta\hat{H}_0(\lambda(0))\}$ being the partition function of the quantum system at time 0. At time 0, the contact between the system and the heat bath is turned off or kept at a negligible level and the system evolves during time interval $[0, \tau]$ according to the force protocol $\lambda(t)$. Here the work done to the system would be a random quantity. Let

$$p_{\tau,0}(W) = \sum_{m,n} Z_0^{-1} e^{-\beta E_n^0} p_{m|n} \delta(W - (E_m^\tau - E_n^0)) \tag{2.8}$$

represent the probability density of work distribution when the system evolves from time 0 to $\tau$. In equation (2.8), $p_{m|n}$ is the probability that the instantaneous eigenstate $|n_{\lambda(0)}\rangle$ at time 0 transits to the instantaneous eigenstate $|m_{\lambda(\tau)}\rangle$ after the evolution. An explicit expression for the transition probability is

$$p_{m|n} = |\langle m_{\lambda(\tau)}|\hat{U}_{\tau,0}|n_{\lambda(0)}\rangle|^2, \tag{2.9}$$

where $\hat{U}_{\tau,0}$ is a unitary operator which characterizes the evolution of the system.

To derive the quantum version of Jarzynski equality, we introduce the characteristic function [16] established by Talkner *et al*:

$$G_{\tau,0}(u) = \int dW e^{iuW} p_{\tau,0}(W), \tag{2.10}$$

which is simply the Fourier transform of the probability density. Starting from this characteristic function, we could write it as a quantum correlation function of $e^{iu\hat{H}_0(\lambda(\tau))}$ and $e^{-iu\hat{H}_0(\lambda(0))}$. It works in the following way:

$$\begin{aligned} G_{\tau,0}(u) &= \sum_{m,n} e^{iuW} p_{\tau,0}(W) \\ &= \sum_{m,n} Z_0^{-1} e^{iu(E_m^\tau - E_n^0)} \langle m_{\lambda(\tau)}|\hat{U}_{\tau,0}|n_{\lambda(0)}\rangle\langle n_{\lambda(0)}|\hat{U}_{\tau,0}^\dagger|m_{\lambda(\tau)}\rangle e^{-\beta E_n^0} \\ &= \sum_{m,n,k} Z_0^{-1} \langle k_{\lambda(0)}|\hat{U}_{\tau,0}^\dagger|m_{\lambda(\tau)}\rangle e^{iuE_m^\tau} \langle m_{\lambda(\tau)}|\hat{U}_{\tau,0}|n_{\lambda(0)}\rangle e^{-iuE_n^0} \langle n_{\lambda(0)}|k_{\lambda(0)}\rangle e^{-\beta E_n^0} \\ &= Tr\{\hat{U}_{\tau,0}^\dagger \sum_m |m_{\lambda(\tau)}\rangle e^{iuE_m^\tau} \langle m_{\lambda(\tau)}|\hat{U}_{\tau,0} \sum_n |n_{\lambda(0)}\rangle e^{-iuE_n^0} \langle n_{\lambda(0)}| \frac{e^{-\beta E_n^0}}{Z_0}\}. \end{aligned}$$

The summation over "$m$" and "$n$" can be written as the exponential of the Hamiltonian at time $\tau$ and time 0. Thus the result above could be expressed as

$$G_{\tau,0}(u) = Z_0^{-1} Tr\{\hat{U}_{\tau,0}^\dagger e^{iu\hat{H}_0(\lambda(\tau))} \hat{U}_{\tau,0} e^{-iu\hat{H}_0(\lambda(0))} e^{-\beta\hat{H}_0(\lambda(0))}\}. \tag{2.11}$$

We emerge $e^{-iu\hat{H}_0(\lambda(0))}$ and $e^{-\beta\hat{H}_0(\lambda(0))}$ into one factor and introduce the parameter $v = -u + i\beta$. By expressing $u$ as $-v + i\beta$, equation (2.11) becomes

$$Z_0 G_{\tau,0}(u) = Tr\{\hat{U}_{\tau,0} e^{iv\hat{H}_0(\lambda(0))} \hat{U}_{\tau,0}^\dagger e^{-iv\hat{H}_0(\lambda(\tau))} e^{-\beta\hat{H}_0(\lambda(\tau))}\}, \tag{2.12}$$

where we have used the property $Tr(\mathbf{AB}) = Tr(\mathbf{BA})$. If we look at the time reversed process, the evolution operator would be $\hat{U}_{0,\tau}$. It is easy to see that $\hat{U}_{\tau,0}^\dagger = \hat{U}_{\tau,0}^{-1} = \hat{U}_{0,\tau}$ because of the unitary property of the time evolution operator. The equation also hold for $\hat{U}_{\tau,0}$ and $\hat{U}_{0,\tau}^\dagger$. Replacing the time evolution operators

in equation (2.12) with time reversed evolution operators, we obtain

$$\begin{aligned} G_{\tau,0}(u) &= Z_0^{-1} Tr\{\hat{U}_{0,\tau}^{\dagger} e^{iv\hat{H}_0(\lambda(0))} \hat{U}_{0,\tau} e^{-iv\hat{H}_0(\lambda(\tau))} e^{-\beta\hat{H}_0(\lambda(\tau))}\} \\ &= Z_0^{-1} Z_\tau G_{0,\tau}(v) \\ &= \frac{Z_\tau}{Z_0} G_{0,\tau}(-u + i\beta). \end{aligned} \tag{2.13}$$

From the work in section 2.1, the ratio of the canonical partition functions could be expressed as $Z_\tau/Z_0 = \exp(-\beta\Delta F)$ where $\Delta F$ is the free energy difference between the two systems at thermal equilibrium. We notice that $G_{0,\tau}(-u+i\beta)$ is exactly a characteristic function of work. Here, the initial state of the system is the equilibrium thermal state $\rho(\tau) = e^{-\beta\hat{H}_0(\lambda(\tau))}/Z_\tau$ and undergoes the evolution described by the time reversed operator $\hat{U}_{0,\tau}$. Knowing $G_{0,\tau}(-u+i\beta) = \int dW e^{iuW} e^{\beta W} p_{0,\tau}(-W)$ where $p_{0,\tau}(-W)$ is the probability density of work done to the system during the time reversed process, we could easily obtain the relation

$$p_{\tau,0}(W) = e^{-\beta\Delta F} e^{\beta W} p_{0,\tau}(-W), \tag{2.14}$$

by taking the inverse Fourier transform on both sides. Equation (2.14) is know as fluctuation theorem or Crooks relation [3]. If we multiply both side of equation (2.14) by $e^{-\beta W}$ and take the summation over all possible work, we would obtain the quantum Jarzynski equality:

$$\langle e^{-\beta W} \rangle = e^{-\beta\Delta F}. \tag{2.15}$$

From the work above, the validity of Jarzynski equality is theoretically verified in quantum systems under unitary evolution. In a recent work [10], experimentalists realized the experimental verification of fluctuation relations at the full quantum level.

# Chapter 3

# Fast-forward Adiabatic Theorem

In a time dependent system, an initial instantaneous eigenstate can make transitions to other instantaneous eigenstates during the evolution process. That is, for an initial state prepared in the instantaneous eigenstate state $|n_{\lambda(0)}\rangle$ of the system at time 0, after the process, the state may fall on the instantaneous eigenstate $|m_{\lambda(\tau)}\rangle (m \neq n)$ of the system at time $\tau$. Such kind of processes are called non-adiabatic process. In many cases, non-adiabatic process complicates the problem because of the transitions and we want to avoid these transitions. Fortunately, adiabatic process could eliminate such kind of transitions and make things easier.

The adiabatic theorem says a physical system remains in its instantaneous eigenstate if a given perturbation is acting on it slowly enough and if there is a gap between the eigenenergy and the rest spectrum of the Hamiltonian [17]. Such kind of process is called adiabatic approximation because the transitions between instantaneous eigenstates is not strictly forbidden. One disadvantage of adiabatic approximation is that it takes a long time to realize. To accelerate the process and maintain adiabatic result at the same time, physicists raised the idea of fast-forward adiabatic process or short-cuts to adiabaticity [18–20]. In our work, we follow Berry's approach of transitionless quantum driving.

In this chapter, we will review the adiabatic approximation and the idea of fast-forward process in quantum systems.

## 3.1 Adiabatic Approximation

We consider a quantum system whose Hamiltonian is described $\hat{H}_0(\lambda(t))$ where $\lambda(t)$ specifies the time dependence of the Hamiltonian. The instantaneous eigenstate at time $t$ is given by

$$\hat{H}_0(\lambda(t))|n_{\lambda(t)}\rangle = E_n(\lambda(t))|n_{\lambda(t)}\rangle, \tag{3.1}$$

with $E_n(\lambda(t))$ being the eigenenergy. Let $|\Psi(t)\rangle$ be the evolving state at time $t$ and it can be expressed in the basis of the instantaneous eigenstates as

$$|\Psi(t)\rangle = \sum_n |n_{\lambda(t)}\rangle\langle n_{\lambda(t)}|\Psi(t)\rangle = \sum_n C_n(t)|n_{\lambda(t)}\rangle. \tag{3.2}$$

The evolution of the state is described by the Schrödinger equation

$$i\hbar\frac{\partial|\Psi(t)\rangle}{\partial t} = \hat{H}_0(\lambda(t))|\Psi(t)\rangle. \tag{3.3}$$

To solve the Schrödinger equation and obtain the explicit expression for $|\Psi(t)\rangle$, we plug (3.2) into euqation (3.3). The equation becomes

$$i\hbar\frac{\partial\sum_n C_n(t)|n_{\lambda(t)}\rangle}{\partial t} = \hat{H}_0(\lambda(t))\sum_n C_n(t)|n_{\lambda(t)}\rangle;$$

$$i\hbar\sum_n(\frac{\partial C_n(t)}{\partial t}|n_{\lambda(t)}\rangle + C_n(t)|\partial_t n_{\lambda(t)}\rangle) = \sum_n E_n(\lambda(t))C_n(t)|n_{\lambda(t)}\rangle. \tag{3.4}$$

In equation (3.4) and subsequent equations, $\partial_t$ represents the derivative with respect to time $t$ for short. If we multiply both sides of equation (3.4) by an arbitrary eigenstate $\langle m_{\lambda(t)}|$, the equation becomes

$$i\hbar\frac{\partial C_m(t)}{\partial t} + i\hbar\sum_n C_n(t)\langle m_{\lambda(t)}|\partial_t n_{\lambda(t)}\rangle = E_m(\lambda(t))C_m(t). \tag{3.5}$$

To re-express $\langle m_{\lambda(t)}|\partial_t n_{\lambda(t)}\rangle$, we differentiate equation (3.1) on both sides and obtains

$$\partial_t\hat{H}_0(\lambda(t))|n_{\lambda(t)}\rangle + \hat{H}_0(\lambda(t))|\partial_t n_{\lambda(t)}\rangle = \partial_t E_n(\lambda(t))|n_{\lambda(t)}\rangle + E_n(\lambda(t))|\partial_t n_{\lambda(t)}\rangle. \tag{3.6}$$

Multiplying equation (3.6) by $\langle m_{\lambda(t)}|$ with the restriction $m \neq n$ gives us

$$\langle m_{\lambda(t)}|\partial_t n_{\lambda(t)}\rangle = \frac{\langle m_{\lambda(t)}|\partial_t \hat{H}_0(\lambda(t))|n_{\lambda(t)}\rangle}{E_n(\lambda(t)) - E_m(\lambda(t))}. \tag{3.7}$$

For non-degenerate system, $m \neq n$ guarantees the denominator $E_n(\lambda(t)) - E_m(\lambda(t)) \neq 0$. With equation (3.7), the expression $\sum_n C_n(t)\langle m_{\lambda(t)}|\partial_t n_{\lambda(t)}\rangle$ could be split into two parts, $C_m(t)\langle m_{\lambda(t)}|\partial_t m_{\lambda(t)}\rangle$ and $\sum_{m\neq n} C_n(t)\langle m_{\lambda(t)}|\partial_t n_{\lambda(t)}\rangle$. Plugging equation (3.7) into equation (3.5)

$$\dot{C}_m(t) = -C_m(t)\langle m_{\lambda(t)}|\partial_t m_{\lambda(t)}\rangle - \sum_{m\neq n} C_n(t)\frac{\langle m_{\lambda(t)}|\partial_t \hat{H}_0(\lambda(t))|n_{\lambda(t)}\rangle}{E_n(\lambda(t)) - E_m(\lambda(t))} - \frac{i}{\hbar}E_m(\lambda(t))C_m(t). \tag{3.8}$$

In adiabatic approximation, the time derivative of the time dependent parameter $\dot{\lambda}$ approaches 0 compared with the energy gap $E_n(\lambda(t)) - E_m(\lambda(t))$ and $\partial_t \hat{H}_0(\lambda(t)) = \dot{\lambda}\partial_\lambda \hat{H}(\lambda)$, hence the second term on the right hand side of equation (3.8) reduces to 0. Solve for $C_m(t)$ gives

$$C_m(t) = C_m(0)e^{-\frac{i}{\hbar}\int_0^t E_m(\lambda(t'))dt' - \int_0^t \langle m_{\lambda(t')}|\partial_{t'} m_{\lambda(t')}\rangle dt'}, \tag{3.9}$$

where $\langle m_{\lambda(t)}|\partial_t m_{\lambda(t)}\rangle$ is pure imaginary. Thus $|C_m(t)|^2 = |C_m(0)|^2$. As $|C_m(t)|$ does not change over time, probability distribution of the eigenstates would not change hence there is no transition from an instantaneous eigenstate $|n_{\lambda(0)}\rangle$ to another instantaneous eigenstate $|m_{\lambda(t)}\rangle$ if $m \neq n$. In equation (3.9), the first part in the exponential which contains $E_m(\lambda(t))$ is the dynamic phase and the second part is called geometric phase and when the evolution is cyclic, we obtain the famous Berry phase.

We now look at the special case when the initial state is prepared in an instantaneous eigenstate of the system at time 0, $|\Psi(0)\rangle = |n_{\lambda(0)}\rangle$. After time $t$, the state remains in the instantaneous eigenstate $|n_{\lambda(t)}\rangle$ and it will be dressed with a dynamic phase and a geometric phase. An explicit expression reads

$$|\Psi(t)\rangle = e^{-\frac{i}{\hbar}\int_0^t dt' E_n(\lambda(t')) - \int_0^t dt' \langle n_{\lambda(t')}|\partial_{t'} n_{\lambda(t')}\rangle}|n_{\lambda(t)}\rangle. \tag{3.10}$$

Equation (3.10) is an important result and it will be used in the next section to deduce the fast-forward process.

## 3.2 Fast-forward Adiabatic process

As the name of fast-forward adiabatic process suggests, it enables us to maintain the adiabatic output for fast changing driven Hamiltonian $\hat{H}_0(\lambda(t))$, even when the system experiences a fast switch. There are two kinds of fast-forward adiabatic process. For a state initialized in the eigenstate $|n_{\lambda(0)}\rangle$, one guarantees that the system stays in $|n_{\lambda(t)}\rangle$ during the whole driving process and the other only ensures the system is in $|n_{\lambda(t)}\rangle$ at the end of the process while in between, transitions between instantaneous eigenstates can happen. The fast-forward method introduced in this article would be the first kind and we follow the approach of transitionless quantum driving where a control Hamiltonian is added to suppress the transitions.

We will consider an arbitrary time-dependent Hamiltonian $\hat{H}_0(\lambda(t))$ whose instantaneous eigenstate is $|n_{\lambda(t)}\rangle$ with energy $E_n(\lambda(t))$ and the state driven by Hamiltonian $\hat{H}_0(\lambda(t))$ is initially prepared in an eigenstate, $|\Psi(t)\rangle = |n_{\lambda(0)}\rangle$. From adiabatic approximation, we know the state driven by slowly changing $\hat{H}_0(\lambda(t))$ at time $t$ is given by equation (3.10). In the fast-forward adiabatic process, we obtain the same result when the state is driven by $\hat{H}(\lambda(t)) = \hat{H}_0(\lambda(t)) + \hat{H}_1(\lambda(t))$ with $\hat{H}_1(\lambda(t))$ being the control Hamiltonian we wish to find. Here, the restriction that $\hat{H}_0(\lambda(t))$ is changing slowly is removed. $|\Psi(t)$ and $\hat{H}(\lambda(t))$ should satisfy the Schrödinger equation:

$$i\hbar\partial_t|\Psi(t)\rangle = \hat{H}(\lambda(t))|\Psi(t)\rangle. \tag{3.11}$$

Let $\hat{U}(t)$ be the unitary time evolution operator. With the state initialized in eigenstate $|n(0)\rangle$, we have

$$\begin{aligned} |\Psi(t)\rangle &= \hat{U}(t)|n_{\lambda(0)}\rangle \\ &= e^{-\frac{i}{\hbar}\int_0^t dt' E_n(\lambda(t')) - \int_0^t dt' \langle n_{\lambda(t')}|\partial_{t'} n_{\lambda(t')}\rangle}|n_{\lambda(t)}\rangle, \end{aligned} \tag{3.12}$$

where "$n$" is arbitrarily chosen. This means, for any specified state $|n_{\lambda(0)}\rangle$ and $|n_{\lambda(t)}\rangle$, equation (3.12) should hold. Hence, the evolution operator would be

$$\hat{U}(t) = \sum_n \exp\left\{-\frac{i}{\hbar}\int_0^t dt' E_n(\lambda(t')) - \int_0^t dt' \langle n_{\lambda(t')}|\partial_{t'} n_{\lambda(t')}\rangle\right\}|n_{\lambda(t)}\rangle\langle n_{\lambda(0)}|. \tag{3.13}$$

Substituting $|\Psi(t)\rangle = \hat{U}(t)|n_{\lambda(0)}\rangle$ into equation (3.11), the $|n_{\lambda(0)}\rangle$ on both sides can be emitted as it is arbitrary. What is left is an equation relating $\hat{U}(t)$ and

$\hat{H}(t)$ and it reads

$$i\hbar\partial_t\hat{U}(t) = \hat{H}(\lambda(t))\hat{U}(t). \tag{3.14}$$

Thus the total Hamiltonian is expressed as

$$\hat{H}(\lambda) = i\hbar(\partial_t\hat{U}(t))\hat{U}^\dagger(t). \tag{3.15}$$

From equation (3.13) and equation (3.15), $\hat{H}(\lambda(t))$ is calculated to be

$$\begin{aligned}
\hat{H}(\lambda(t)) &= i\hbar\partial_t \sum_n \exp\left\{-\frac{i}{\hbar}\int_0^t dt' E_n(\lambda(t')) - \int_0^t dt'\langle n_{\lambda(t')}|\partial_{t'} n_{\lambda(t')}\rangle\right\} |n_{\lambda(t)}\rangle\langle n_{\lambda(0)}| \\
&\qquad \sum_m \exp\left\{\frac{i}{\hbar}\int_0^t dt' E_m(\lambda(t')) + \int_0^t dt'\langle m_{\lambda(t')}|\partial_{t'} m_{\lambda(t')}\rangle\right\} |m_{\lambda(0)}\rangle\langle m_{\lambda(t)}| \\
&= \sum_n i\hbar\left[\left(-\frac{i}{\hbar}E_n(\lambda(t)) - \langle n_{\lambda(t)}|\partial_t n_{\lambda(t)}\rangle\right)|n_{\lambda(t)}\rangle + |\partial_t n_{\lambda(t)}\rangle\right]\langle n_{\lambda(t)}| \\
&= i\hbar\sum_n(|\partial_t n_{\lambda(t)}\rangle\langle n_{\lambda(t)}| - \langle n_{\lambda(t)}|\partial_t n_{\lambda(t)}\rangle|n_{\lambda(t)}\rangle\langle n_{\lambda(t)}|) \\
&\qquad + \sum_n |n_{\lambda(t)}\rangle E_n(\lambda(t))\langle n_{\lambda(t)}|.
\end{aligned} \tag{3.16}$$

It should be noticed that $\int_0^t dt'\langle n_{\lambda(t')}|\partial_{t'} n_{\lambda(t')}\rangle$ is a pure imaginary number so that the exponential terms cancel out. As $\hat{H}(\lambda(t)) \equiv \hat{H}_0(\lambda(t)) + \hat{H}_1(\lambda(t))$ and it is easy to see $\sum_n |n_{\lambda(t)}\rangle E_n(\lambda(t))\langle n_{\lambda(t)}| = \hat{H}_0(\lambda)$, the control Hamiltonian we are looking is exactly:

$$\begin{aligned}
\hat{H}_1(\lambda(t)) &= i\hbar\sum_n(|\partial_t n_{\lambda(t)}\rangle\langle n_{\lambda(t)}| - \langle n_{\lambda(t)}|\partial_t n_{\lambda(t)}\rangle|n_{\lambda(t)}\rangle\langle n_{\lambda(t)}|) \\
&= i\hbar\sum_n\left(\sum_m\langle m_{\lambda(t)}|\partial_t n_{\lambda(t)}\rangle|m_{\lambda(t)}\rangle\langle n_{\lambda(t)}| - \langle n_{\lambda(t)}|\partial_t n_{\lambda(t)}\rangle|n_{\lambda(t)}\rangle\langle n_{\lambda(t)}|\right) \\
&= i\hbar\sum_n\sum_{m\neq n}|m_{\lambda(t)}\rangle\langle m_{\lambda(t)}|\partial_t n_{\lambda(t)}\rangle\langle n_{\lambda(t)}|.
\end{aligned} \tag{3.17}$$

For non-degenerate system, $\langle m_{\lambda(t)}|\partial_t n_{\lambda(t)}\rangle$ is given by equation (3.7). The control Hamiltonian can thus be written in the form

$$\hat{H}_1(\lambda) = i\hbar\sum_n\sum_{m\neq n}\frac{|m_{\lambda(t)}\rangle\langle m_{\lambda(t)}|\partial_t\hat{H}_0(\lambda(t))|n_{\lambda(t)}\rangle\langle n_{\lambda(t)}|}{E_n(\lambda(t)) - E_m(\lambda(t))}. \tag{3.18}$$

An immediate check on the expression is that when the Hamiltonian $\hat{H}_0(\lambda(t))$ is time independent or is changing slowly enough compared with the energy gap

$E_n(\lambda(t)) - E_m(\lambda(t))(m \neq n)$ (this is exactly the condition for adiabatic approximation to be valid), the control Hamiltonian takes the value 0 or approaches 0 as expected.

By adding an appropriate external Hamiltonian to the original driving Hamiltonian, we eliminate the transitions between instantaneous eigenstates (quantum number does not change) when the system undergoes fast evolution, hence realize the idea of fast-forward adiabatic process. The fast-forward adiabatic process will be applied to two-level system and quantum harmonic oscillator for detailed study on the convergence of Jarzynski equality.

# Chapter 4

# Two-Level System

Two-level system is the most fundamental and simple quantum system. It can be used to describe the polarization of photons and spin - $\frac{1}{2}$ particles. Because of its simplicity, two-level systems are frequently used by physicists. Theoreticians often use two-level systems for theory development and experimentalists often use it for verification of the theories developed by theoreticians. The most famous experiment on a two-level system would be the Stern-Gerlach Experiment in 1922. It is an important experiment in quantum mechanics on the deflection of particles and can be used to demonstrate that electrons and atoms have intrinsic quantum properties and how measurement in quantum mechanics affects the system being measured.

To investigate the Jarzynski equality, we also take two-level system as our work frame. In our research, the fast-forward adiabatic process is applied to an evolving two-level system to see the impact of fast-forward process on the convergence of Jarzynski equality and to study the details of Jarzynski equality including how changes of temperature and negative works affect the convergence.

This chapter shows our investigation on two-level system. It starts with a description of a two-level system considered and followed by the results of simulated evolutions under non-adiabatic and fast-forward adiabatic process at different temperatures. Comparisons and analysis are made to illustrate how fast-forward adiabatic process make a difference in the convergence of Jarzynski equality and the roles that temperature and negative works play during the convergence.

## 4.1 Fast-forward Adiabatic Process on Two-Level System

### 4.1.1 Description of a Two-Level System

We consider the Landau-Zener transition model with the following Hamiltonian:

$$\begin{aligned}\hat{H}_0(\lambda(t)) &= \begin{pmatrix} \lambda(t) & \triangle \\ \triangle & -\lambda(t) \end{pmatrix} \\ &= \lambda(t)\sigma^z + \triangle\, \sigma^x, \end{aligned} \tag{4.1}$$

where $\lambda(t)$ is the time dependent parameter specifying the time dependence of $\hat{H}_0(\lambda(t))$, $\triangle$ is a constant and $\sigma^{x,y,z}$ are the usual Pauli Matrices. We use the eigenstates of $\sigma^z$ as our orthogonal basis so that

$$|+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}; \qquad |-\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

For a general $\overrightarrow{S} = \sin\theta\cos\phi\sigma^x + \sin\theta\sin\phi\sigma^y + \cos\theta\sigma^z$, its eigenvector is given by

$$|+n\rangle = \cos\frac{\theta}{2}|+\rangle + \sin\frac{\theta}{2}e^{i\phi}|-\rangle;$$

$$|-n\rangle = \sin\frac{\theta}{2}|+\rangle + \cos\frac{\theta}{2}e^{i(\phi+\pi)}|-\rangle.$$

In our Landau-Zener transition model, the $y$ component is missing so that $\phi = 0$. Write the Hamiltonian as

$$\hat{H}_0(\lambda(t)) = \sqrt{\lambda^2(t) + \triangle^2}(\sin 2\theta\sigma^x + \cos 2\theta\sigma^z),$$

with $\theta$ obeying

$$\sin 2\theta = \frac{\triangle}{\sqrt{\lambda^2(t) + \triangle^2}}; \qquad \cos 2\theta = \frac{\lambda(t)}{\sqrt{\lambda^2(t) + \triangle^2}}. \tag{4.2}$$

Hence it is easy to obtain the instantaneous eigenstates of the Hamiltonian as

$$\begin{aligned} |1_{\lambda(t)}\rangle &= \sin\theta|+\rangle - \cos\theta|-\rangle \\ |2_{\lambda(t)}\rangle &= \cos\theta|+\rangle + \sin\theta|-\rangle, \end{aligned} \tag{4.3}$$

and the energy for $|1_{\lambda(t)}\rangle$ is $E_1(\lambda(t)) = -\sqrt{\triangle^2 + \lambda^2(t)}$; energy for $|2_{\lambda(t)}\rangle$ is $E_2(\lambda(t)) = \sqrt{\triangle^2 + \lambda^2(t)}$

### 4.1.2 The Control Hamiltonian $\hat{H}_1(\lambda(t))$

We perform fast-forward adiabatic driving on a two-level system. With all the details of the two-level system described in section 4.1.1 and the general expression of control Hamiltonian in equation (3.18) derived in section 3.2, the control Hamiltonian $\hat{H}_1(\lambda(t))$ is solved as follows:

$$
\begin{aligned}
\hat{H}_1(\lambda(t)) &= i\hbar \sum_n \sum_{m \neq n} \frac{|m_{\lambda(t)}\rangle\langle m_{\lambda(t)}|\partial_t \hat{H}_0(\lambda(t))|n_{\lambda(t)}\rangle\langle n_{\lambda(t)}|}{E_n(\lambda(t)) - E_m(\lambda(t))} \\
&= i\hbar \frac{|1_{\lambda(t)}\rangle\langle 1_{\lambda(t)}|\partial_t \hat{H}_0(\lambda(t))|2_{\lambda(t)}\rangle\langle 2_{\lambda(t)}|}{E_2(\lambda(t)) - E_1(\lambda(t))} + \\
&\qquad\qquad i\hbar \frac{|2_{\lambda(t)}\rangle\langle 2_{\lambda(t)}|\partial_t \hat{H}_0(\lambda(t))|1_{\lambda(t)}\rangle\langle 1_{\lambda(t)}|}{E_1(\lambda(t)) - E_2(\lambda(t))} \\
&= i\hbar \left( \frac{|1_{\lambda(t)}\rangle\langle 1_{\lambda(t)}|\dot{\lambda}(t)\sigma^z|2_{\lambda(t)}\rangle\langle 2_{\lambda(t)}|}{2\sqrt{\triangle^2 + \lambda^2(t)}} - \frac{|2_{\lambda(t)}\rangle\langle 2_{\lambda(t)}|\dot{\lambda}(t)\sigma^z|1_{\lambda(t)}\rangle\langle 1_{\lambda(t)}|}{2\sqrt{\triangle^2 + \lambda^2(t)}} \right) \\
&= i\hbar \frac{\dot{\lambda}(t)}{2\sqrt{\triangle^2 + \lambda^2(t)}} \begin{pmatrix} \sin\theta \\ -\cos\theta \end{pmatrix} (\sin\theta \quad -\cos\theta) \begin{pmatrix} \cos\theta \\ -\sin\theta \end{pmatrix} (\cos\theta \quad \sin\theta) \\
&\qquad - \begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix} (\cos\theta \quad \sin\theta) \begin{pmatrix} \sin\theta \\ \cos\theta \end{pmatrix} (\sin\theta \quad -\cos\theta) \\
&= \frac{i\hbar\dot{\lambda}(t)\sin 2\theta}{2\sqrt{\triangle^2 + \lambda^2(t)}} \left[ \begin{pmatrix} \sin\theta\cos\theta & \sin^2\theta \\ -\cos^2\theta & \sin\theta\cos\theta \end{pmatrix} - \begin{pmatrix} \sin\theta\cos\theta & -\cos^2\theta \\ \sin^2\theta & \sin\theta\cos\theta \end{pmatrix} \right] \\
&= i\hbar\dot{\lambda}(t) \frac{1}{2} \frac{\triangle}{\triangle^2 + \lambda^2(t)} \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \\
&\equiv -\hbar\dot{\lambda}(t) \frac{1}{2} \frac{\triangle}{\triangle^2 + \lambda^2(t)} \sigma^y. \qquad (4.4)
\end{aligned}
$$

Note that the control Hamiltonian is proportional to the time derivative of the time-dependent parameter $\lambda(t)$. Hence, it reduces to 0 when $\lambda(t)$ changes slowly which recovers the adiabatic approximation.

### 4.1.3 Thermal Ensemble

As mentioned, the initial state is prepared in equilibrium thermal state which could be achieved by keeping the system in contact with a heat bath with inverse temperature $\beta$ till time $t = 0$. Hence the initial state is given by equation (2.7)

$$\rho(0) \equiv \frac{1}{Z_0} e^{-\beta \hat{H}_0(\lambda(0))} = \sum_n \frac{e^{-\beta E_n(\lambda(0))}}{Z_0} |n_{\lambda(0)}\rangle\langle n_{\lambda(0)}|, \tag{4.5}$$

where $Z_0$ is the partition function of the ensemble at time 0 and is given by

$$Z_0 = Tr\left\{e^{-\beta \hat{H}_0(\lambda(0))}\right\} = \sum_n e^{-\beta E_n(\lambda(0))}. \tag{4.6}$$

Equation (4.5) and (4.6) is a general expression of the equilibrium thermal state and it will also be applied to the Harmonic Oscillator systems latter in Chapter 5. Here explicit for the two-level system with energy $\pm\sqrt{\triangle^2 + \lambda^2(t)}$, the initial state would be

$$\rho(0) = \frac{e^{-\sqrt{\triangle^2+\lambda^2(t)}}}{Z_0} |1_{\lambda(0)}\rangle\langle 1_{\lambda(0)}| + \frac{e^{\sqrt{\triangle^2+\lambda^2(t)}}}{Z_0} |2_{\lambda(0)}\rangle\langle 2_{\lambda(0)}|,$$
$$Z_0 = e^{-\sqrt{\triangle^2+\lambda^2(t)}} + e^{\sqrt{\triangle^2+\lambda^2(t)}}.$$

For evolution from time $0 \to \tau$, work function is given by equation (2.8). In fast-forward adiabatic process, transitions between energy levels are suppressed such that $p_{m|n} = \delta_{mn}$ and

$$P(W) = \sum_n e^{-\beta E_n(0)}/Z(0)\delta(W - [E_n(\tau) - E_n(0)]). \tag{4.7}$$

## 4.2 Numerical Simulations on Two-Level System

We design the protocol so that the control Hamiltonian $\hat{H}_1(\lambda(t))$ vanishes both at the beginning and the end of the fast-forward process which requires $\dot{\lambda}(0) = \dot{\lambda}(\tau) = 0$. Hence, the work done to the system by the control Hamiltonian $\hat{H}_1(\lambda(t))$ and the original Hamiltonian $\hat{H}_0(\lambda(t))$ is still given by $[E_m(\lambda(\tau)) - E_n(\lambda(0))]$ in a particular two-time projective measurement. The expression of work does not change when the control Hamiltonian is added to the Original Hamiltonian. An

appropriate scheme is

$$\lambda(t) = \lambda_0 \sqrt{\frac{a^2+1}{2} - \frac{a^2-1}{2}\cos(n\pi\frac{t}{\tau})}. \tag{4.8}$$

Parameters are fixed to be: $\lambda_0 = 1, a = 3, \Delta = 2$, $n = 1$ and $\hbar = 1$ and simulations are done under non-adiabatic process and fast-forward adiabatic process.

### 4.2.1 Transitions between Instantaneous Eigenstates

To obtain the probability distribution of work done to the system, we need to know the transition probabilities between instantaneous eigenstates, $p_{m|n}$ and the initial distribution of the state $P_n = \frac{e^{-\beta E_n(\lambda(0))}}{Z_0}$. For a known system, $P_n$ will be immediately known when temperature $\beta$ is specified. In two-level system, there are 4 possible transitions $p_{1|1}, p_{2|1}, p_{1|2}$ and $p_{2|2}$.

To calculate these transition probabilities, the eigenstate $|1_{\lambda(0)}\rangle$ and state $|2_{\lambda(0)}\rangle$ of the system at time 0 are chosen as initial state respectively. For each initial state, we simulate the time evolution of the state driven by $\hat{H}_0(\lambda(t))$ for non-adiabatic process and $\hat{H}(\lambda(t)) = \hat{H}_0(\lambda(t)) + \hat{H}_1(\lambda(t))$ for fast-forward adiabatic process and obtain the corresponding final state $|\psi(\tau)\rangle$. $p_{m|n}$ is given by the probability that state $|\psi(\tau)\rangle$ falls into eigenstate $|m_{\lambda(\tau)}\rangle$ of $\hat{H}_0(\lambda(\tau))$. The worked-out transition probabilities for non-aidabatic process are shown in the table below:

TABLE 4.1: Transition probabilities for two-level system

| | final state $\|1_{\lambda(\tau)}\rangle$ | final state $\|2_{\lambda(\tau)}\rangle$ |
|---|---|---|
| initial state $\|1_{\lambda(0)}\rangle$ | 0.9341 | 0.0659 |
| initial state $\|2_{\lambda(0)}\rangle$ | 0.0659 | 0.9341 |

The transition probabilities do not depend on the temperature as temperature only affects the equilibrium thermal state and does not involve in the evolution. In the simulation, we choose one specific eigenstate as the initial state and $p_{m|n}$ is fully determined by the evolution operator. From table 4.1, we find that under the condition considered for the two-level system, the state will remain in the same energy level with a high probability. It is also noticed that $p_{1|2} = p_{2|1}$, meaning the probability for eigenstate $|1_{\lambda(0)}\rangle$ to transit into eigenstate $|2_{\lambda(\tau)}\rangle$ equals the probability for eigenstate $|2_{\lambda(0)}\rangle$ to transit into eigenstate $|1_{\lambda(\tau)}\rangle$. We call this

transition symmetry. This symmetry is also observed in the study on quantum harmonic oscillators in the latter part of the report.

### 4.2.2 Convergence of Jarzynski Equality in Two-Level System

We simulate the convergence of Jarzynski equality under non-adiabatic and fast-forward adiabatic process. This time the initial state is prepared in the equilibrium thermal state described by equation (4.5) which is a mixture of instantaneous eigenstates of $\hat{H}_0(\lambda(0))$. The simulation is done in the following manner. At time $t = 0$, an energy measurement is performed to the two-level system so that $E_n(\lambda(0))$ is obtained. The system then evolves according to driving Hamiltonian $\hat{H}_0(\lambda(t))$ for non-adiabatic case and $\hat{H}(\lambda(t)) = \hat{H}_0(\lambda(t)) + \hat{H}_1(\lambda(t))$ for fast-forward adiabatic case during time interval $[0, \tau]$. At the end of the process, another energy measurement is performed such that $E_m(\lambda(\tau))$ is also obtained. Hence, the work done to the two-level system is given by $W = E_m(\lambda(\tau)) - E_n(\lambda(0))$. The whole procedure is repeated and we call each repeat one independent trajectory. For the $i^{th}$ $(i = 1, 2, 3 \cdots)$ trajectory, we take the exponential of the work measured to be $e^{-\beta W_i}$ and average $e^{-\beta W}$ over the "N" trajectories completed. In this way, we could view how the averaged exponential of work $\langle e^{-\beta W} \rangle$ converges to its expected value $e^{-\beta \Delta F}$.

To make clear the effect of a temperature change on the convergence, the simulation is done under different temperatures from high to low for comparison. The averaged exponential work $\langle e^{-\beta W} \rangle$ is plotted against the number of trajectories. Figure 4.1 presents the plot when the temperature is set to be very high at $\beta = 0.01$.

For the plot in Figure 4.1 and also for subsequent plots of the convergence of Jarzynski equality in two-level system, we plot one dot for every 10 trajectories. From Figure 4.1, we find that at the extremely high temperature $\beta = 0.01$, no difference is exhibited in the convergence of $\langle e^{-\beta W} \rangle$ between the non-adiabatic and fast-forward adiabatic process. We also notice that in this simulation, the value of $\langle e^{-\beta W} \rangle$ converges to the theoretical value very fast. When we look into the details of the simulation, the values of the exponential of work $e^{-\beta W_{ij}}$ $(i, j = 1, 2)$ are found to be very close to the value of $e^{-\beta \Delta F}$, thus $e^{-\beta W}$ has a very narrow

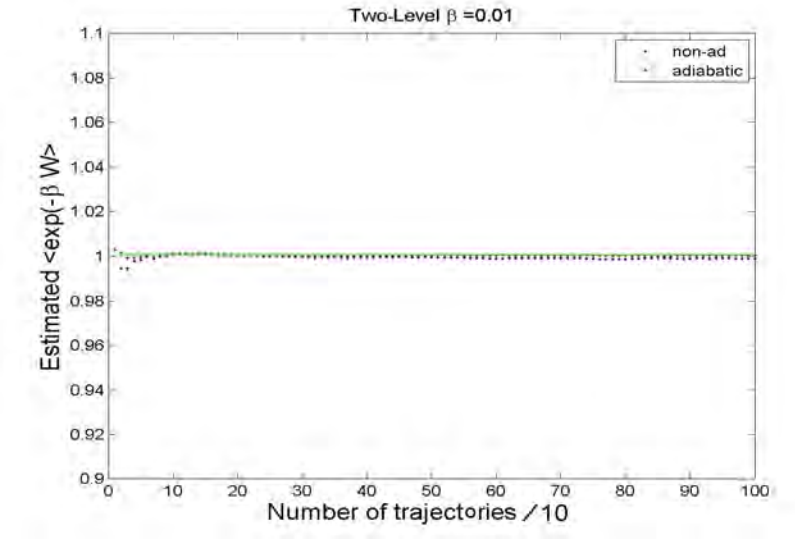


FIGURE 4.1: Simulation of the convergence of $\langle e^{-\beta W} \rangle$ for two-level system at temperature $\beta = 0.01$. The blue dots represent the non-adiabatic process and the red ones represent the fast-forward adiabatic process. The green line is the theoretical value $e^{-\beta \Delta F} = 1.0004$. In the label of the x axis, "/10" means we plot one dot for every 10 trajectories.

probability distribution around its expectation $e^{-\beta \Delta F}$. From our knowledge of statistics, we know such distribution would converge to its expectation very fast.

When the temperature is lowered to $\beta = 0.1$, the convergence tendency of the two processes is plotted in Figure 4.2.

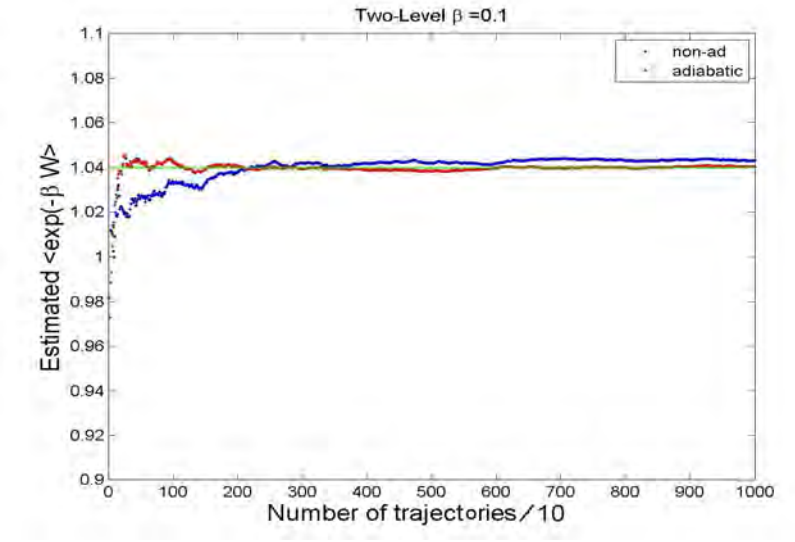


FIGURE 4.2: Simulation of convergence of $\langle e^{-\beta W} \rangle$ at temperature $\beta = 0.1$. The blue dots represent the non-adiabatic process and the red ones represent the fast-forward adiabatic process. The green line is the theoretical value $e^{-\beta \Delta F} = 1.0396$.

At a lower temperature, the result from fast-forward adiabatic process begins to distinguish from the non-adiabatic process. Figure 4.2 shows that under fast-forward adiabatic process, $\langle e^{-\beta W} \rangle$ converges to its expectation around the scale 200 while under non-adiabatic process, $\langle e^{-\beta W} \rangle$ is still slightly different from its expectation when the scale goes to 1000. The convergence of Jarzynski equality is accelerated. It is also noticed that after 2500 $(250 \times 10)$ trajectories, the averaged exponential of work $\langle e^{-\beta W} \rangle$ under non-adiabatic process is very close to the expectation $e^{-\beta \Delta F}$. In this sense, at temperature $\beta = 0.1$, there is some improvement from fast-forward adiabatic process, but not very significant.

When we compare Figure 4.1 and 4.2, it is found that the convergence speed at temperature $\beta = 0.01$ is much faster than the speed at temperature $\beta = 0.1$ under both processes. This is because the value of $e^{-\beta W_{i,j}} (i, j = 1, 2)$ get largely differed from its expectation and the difference between themselves also becomes larger. The spread of the distribution of $e^{-\beta W}$ gets wider, thus resulting in a slower convergence speed. A more detailed analysis on the effect of temperature on the convergence of Jarzynski equality will be carried out when we have more simulation results with different temperatures.

When the temperature is decreased further to $\beta = 0.5$, the simulation of the convergence of Jarzynski equality is presented in Figure 4.3.

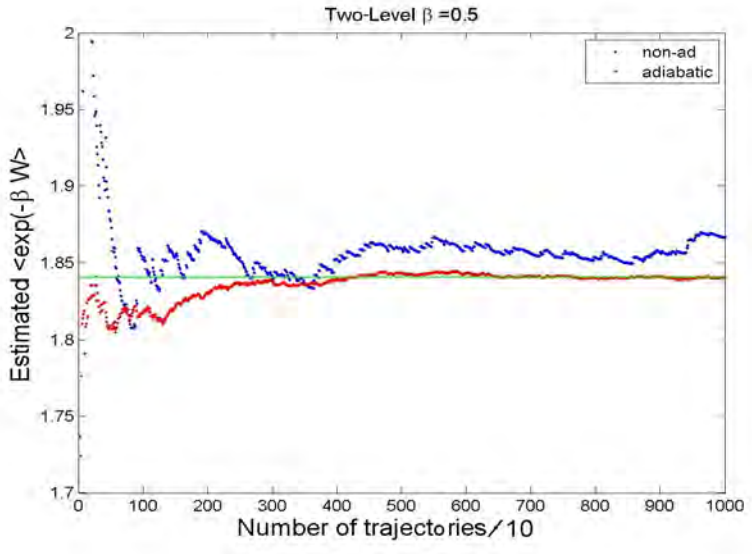


FIGURE 4.3: Simulation of convergence of $\langle e^{-\beta W} \rangle$ at temperature $\beta = 0.5$. The blue dots represent the non-adiabatic process and the red ones represent the fast-forward adiabatic process. The green line is the theoretical value $e^{-\beta \Delta F} = 1.8404$.

When the temperature decreases further, a more distinct result is observed between the convergence under fast-forward adiabatic and non-adiabatic process in Figure 4.3. At $\beta = 0.5$ which we consider to be a moderate temperature, the improvement from fast-forward adiabatic process on the convergence of Jarzynski equality becomes significant. After 3000 ($300 \times 10$) trajectories, we have a very good convergence for the fast-forward adiabatic process and when the process is non-adiabatic, the estimated $\langle e^{-\beta W} \rangle$ is still far from the expectation. It is noticed that in the plot, the convergence for the non-adiabatic process is not observed, but this does not mean that $\langle e^{-\beta W} \rangle$ does not follow Jarzynski equality in this case. The reason is simply we do not have enough trajectories. With more trajectories, $\langle e^{-\beta W} \rangle$ will eventually converge to its expected value and a verification is done with the plot presented in Appendix A for reference. In our subsequent simulations, the same phenomenon may occur due to the same reason.

Another observation from Figure 4.3 is that the convergence for both processes is again slowed down compared with the result presented in Figure 4.2. It seems that at high temperature, $\langle e^{-\beta W} \rangle$ converges very fast and as temperature decreases ($\beta$ gets larger), the convergence of Jarzynski equality becomes poorer. To see whether this statement holds, we did two more simulations for our two-level system at temperature $\beta = 1.0$ and $\beta = 1.5$.

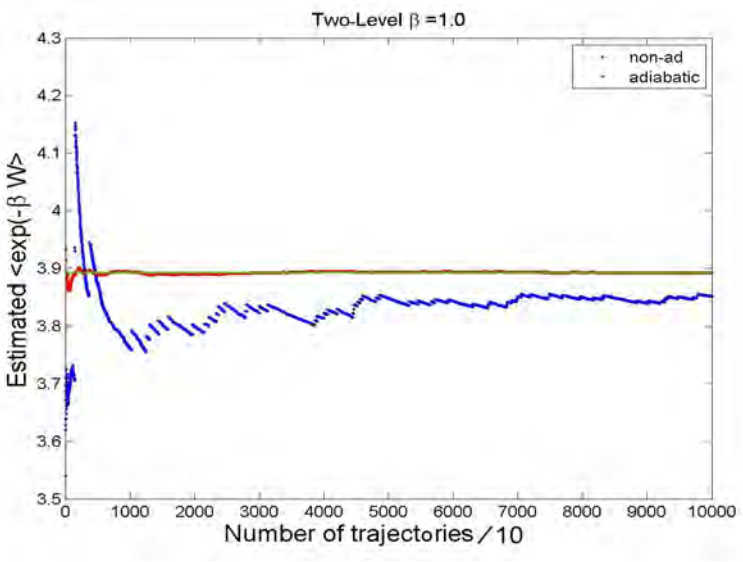


FIGURE 4.4: Simulation of convergence of $\langle e^{-\beta W} \rangle$ at temperature $\beta = 1.0$. The blue dots represent the non-adiabatic process and the red ones represent the fast-forward adiabatic process. The green line is the theoretical value $e^{-\beta \Delta F} = 3.8918$.

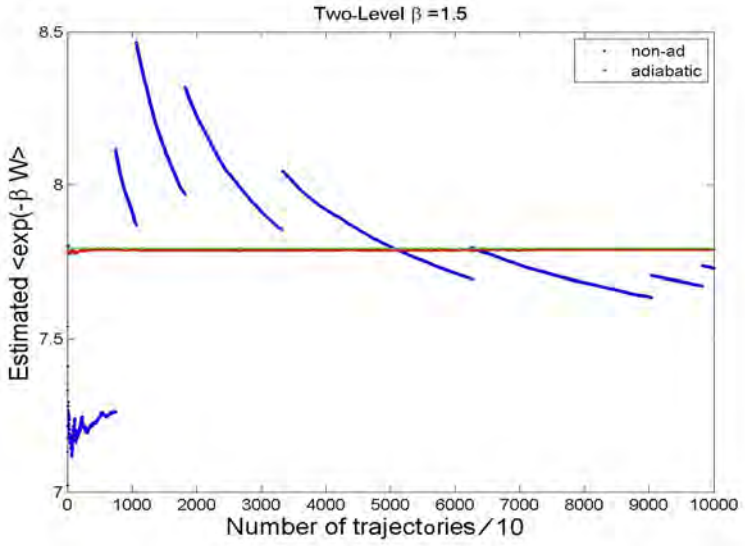


FIGURE 4.5: Simulation of convergence of $\langle e^{-\beta W} \rangle$ at temperature $\beta = 1.5$. The blue dots represent the non-adiabatic process and the red ones represent the fast-forward adiabatic process. The green line is the theoretical value $e^{-\beta \Delta F} = 7.7914$.

In Figure 4.4 and 4.5 when $\beta = 1.0, 1, 5$, the scale of x axis is increased to $10^4$. It is noticed that the difference on the converge speed for two-level system between the two processes gets even larger. When $\beta = 1.0$, $\langle e^{-\beta W} \rangle$ converges after 1500 $(150 \times 10)$ trajectories and when $\beta = 1.5$, $\langle e^{-\beta W} \rangle$ converges to its expected value at the very beginning under fast-forward process. For non-adiabatic process, the convergence is delayed further at a lower temperature (Refer to Appendix A to see the converge speed at $\beta = 0.5, 1.0, 1.5$). Here the effect of temperature on Jarzynski convergence differs for the two different processes.

Another important finding is that under non-adiabatic process, there are some jumps in the plot. Each jump in the plot indicates an extreme value caused by transition from high energy level to low energy level. In our two-level system, when the state transits from hihg energy level to low energy level, it gives us a large negative work and this negative work, after taking the exponential, $e^{-\beta W}$ becomes a huge number compared with other values of $e^{-\beta W}$. The effect of these negative work are reflected in the plot as big jumps.

### 4.2.3 Analysis

From subsection 4.2.2, it is shown that when temperature is high, the convergence of Jarzynski equality in our two-level system under fast-forward adiabatic process is the same with the convergence under a normal non-adiabatic process. As temperature decreases, the results for the two processes become different and the improvement from fast-forward adiabatic process is enlarged when temperature is lowered down. We compare the variance of $e^{-\beta W}$ and the dissipated work $\langle W_{dis} \rangle = \langle W \rangle - \Delta F$ which is defined as the difference between the expected work done to the system and the Helmholtz free energy difference and find:

TABLE 4.2: Variance of $e^{-\beta W}$ and Dissipated work $\langle W_{dis} \rangle$

| | | Variance $[\sigma^2(e^{-\beta W})]$ | Dissipated work $[\langle W_{dis} \rangle]$ |
|---|---|---|---|
| $\beta_1 = 0.01$ | Non-Adiabatic | $3.8156 \times 10^{-4}$ | 0.0200 |
| | Adiabatic | $1.8754 \times 10^{-4}$ | 0.0094 |
| $\beta_2 = 0.1$ | Non-Adiabatic | 0.0412 | 0.1917 |
| | Adiabatic | 0.0179 | 0.0872 |
| $\beta_3 = 0.5$ | Non-Adiabatic | 2.5142 | 0.4983 |
| | Adiabatic | 0.1906 | 0.1150 |
| $\beta_4 = 1.0$ | Non-Adiabatic | 74.1494 | 0.4896 |
| | Adiabatic | 0.1491 | 0.0203 |
| $\beta_5 = 1.5$ | Non-Adiabatic | 285.50 | 0.4764 |
| | Adiabatic | 0.0805 | 0.0025 |

In the table, "adiabatic" refers to the fast-forward adiabatic process. It is noticed that when the process is adiabatic, the variance $\sigma^2(e^{-\beta W})$ and the dissipated work $\langle W_{dis} \rangle$ are smaller compared with that in non-adiabatic case. The smaller variance explains the convergence improvement from fast-forward adiabatic process and the smaller dissipated agrees with the idea in [11] that reduced dissipated work leads to faster convergence of $\langle e^{-\beta W} \rangle$. A more fundamental reason is that non-adiabatic transitions between energy levels are eliminated in adiabatic process. The explanation for larger improvement at lower temperature goes to the effect of temperature and negative works (Remember that we use "negative work" to denote the negative work due to transitions between instantaneous eigenstates for convenience) on the convergence.

We first look at adiabatic case. In the adiabatic case, there is no transition between instantaneous eigenstates so that the probability distribution of $e^{-\beta W}$ is simply the probability distribution of the initial state. For a two-level system, we have only two values of work done to the system in adiabatic process,

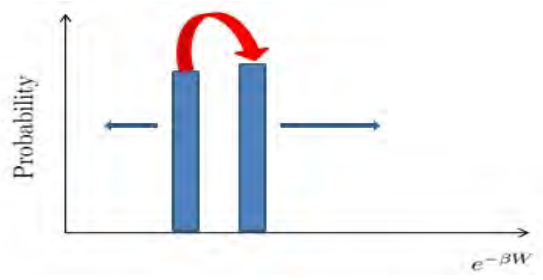


FIGURE 4.6: Change of probability distribution of $e^{-\beta W}$ when $\beta$ increases

$W_{11} = -1.3695, W_{2|2} = 1.3695$. At high temperature, the probability that the initial state is in eigenstate $|1_{\lambda(0)}\rangle$ and $|2_{\lambda(0)}\rangle$ is close. Hence in the simulation, there would be many initial state in both $|1_{\lambda(0)}\rangle$ (gives work $W_{11}$ after the trajectory) and $|2_{\lambda(0)}\rangle$ (gives work $W_{22}$ after the trajectory) after the energy measurement at $t = 0$. For small $\beta$, $e^{-\beta W_{11}}$ and $e^{-\beta W_{22}}$ are close to each other. When temperature decreases, probability weight is shifted to $e^{-\beta W_{11}}$, and the difference between $e^{-\beta W_{11}}$ and $e^{-\beta W_{22}}$ becomes large. The simple diagram in Figure 4.6 describes the situation. Thus an decrease in temperature has two opposite effects. The shift of probability weight makes the convergence faster (effect 1) and the separation of $e^{-\beta W_{11}}$ and $e^{-\beta W_{22}}$ makes the convergence slower (effect 2). When temperature is kept at a relatively high level, effect 2 is the dominant effect which causes a slow-down in the convergence when temperature decreases. When temperature decreases further, effect 1 becomes dominant and the convergence is speeded up.

When the process is non-adiabatic, transitions between instantaneous eigenstates comes into action. Transitions from low energy level to high energy level do not have much effect on the convergence, so we will look at transitions from high energy level to low energy level only which produce negative works. The number of negative work realizations in simulations is 30 out of 1000 for $\beta = 0.01$, 254 out of $10^4$ for $\beta = 0.1$, 57 out of $10^4$ for $\beta = 0.5$, 69 out of $10^5$ for $\beta = 1.0$ and 7 out of $10^5$ for $\beta = 1.5$. From Table 4.2 and the number listed above, we could see the variance of $e^{-\beta W}$ increases rapidly with decreased temperature and the ratio of negative work realization is reduced with lowered temperature. Similar with the situation in fast-forward adiabatic process, the effect of temperature in non-adiabatic process for two-level system also consists of two opposite parts. One is a positive effect due to a more concentrated distribution of initial state and the other is a negative effect due to a wider spread of $e^{-\beta W}$, or to be more exact, the extreme values of $e^{-\beta W}$ caused by the negative work realizations. At high temperatures, these negative work do not cause big trouble as the $e^{-\beta W}$ for negative work realizations

is not very much different from other trajectories. At low temperatures, they increase wildly and become extreme values in the distribution. Although the ratio of negative work realizations decreases and the probability weight is shifted to $e^{-\beta W_{11}}$ with decreased temperature, the variance $\sigma^2(e^{-\beta W})$ is still largely increased and the convergence of Jarzynski equality becomes poorer (To see the convergence at $\beta = 0.5$, $\beta = 1.0$ and $\beta = 1.5$, please refer to Appendix A).

From the above analysis on the simulations, for fast-forward adiabatic process, the convergence of Jarzynski equality is the same with the case in non-adiabatic process at high temperature and is greatly improved at low temperature. The effect of temperature on the convergence is largely reduced in fast-forward adiabatic situation. In the case of fast-forward adiabatic process, the convergence is slowed down with decreased temperature when the temperature is kept at a high level and accelerated with decreased temperature when the temperature is lowered further. In non-adiabatic process, the effect of temperature and the effect of negative work on the convergence of Jarzynski equality come together. At high temperature, negative work do not affect the convergence very much while at low temperature, they lead to a wild increase in the variance of the exponential work, thus greatly slowing down the convergence. Hence the convergence becomes poorer at lower temperature. These results are further checked on quantum harmonics oscillators where the system has infinite energy levels.

# Chapter 5

# Quantum Harmonic Oscillator

Quantum harmonic oscillator is a very important system in quantum mechanics. It can be used to model various situations. For example, the trapped ions are perfectly modelled by oscillators; the quantum heat engine (Quantum Otto cycle) [21] can also be described by harmonics oscillators and in the quantization of electromagnetic field, harmonic oscillator works as the Hamiltonian of the quantized field. To further verify that our idea of fast-forward adiabatic process accelerates the convergence of Jarzynski equality and check the effect of temperature and negative works on the convergence, an investigation on quantum harmonic oscillator system is carried out.

In this chapter, we present our studies on the harmonic oscillator system. We first review how the fast-forward adiabatic could be achieved on a quantum harmonic oscillator and then do a series of simulations for non-adiabatic process and fast-forward adiabatic process at various temperatures. By analysing and comparing these results from the simulations, we verify the efficiency of the fast-forward adiabatic method and the effect of temperature and negative works on the convergence of Jarzynski equality

## 5.1 Fast-forward Adiabatic Process on Quantum Harmonic Oscillator

### 5.1.1 Description of The Harmonic Oscillator

We use Berry's transitionless quantum driving to achieve our fast-forward adiabatic process. As it requires the system to be non-degenerate, we consider a 1-D harmonic oscillator with time-dependent frequency $\omega(t)$. Here $\omega(t)$ acts as the time-dependent parameter $\lambda(t)$. The Hamiltonian is given by:

$$\hat{H}_0(\omega(t)) = \frac{\hat{p}^2}{2m} + \frac{m\omega^2(t)\hat{q}^2}{2}. \tag{5.1}$$

The eigenstates and energy obey the relation:

$$\hat{H}_0(\omega(t))|n_{\omega(t)}\rangle \equiv E_n(\omega(t))|n_{\omega(t)}\rangle = (n+\frac{1}{2})\hbar\omega(t)|n_{\omega(t)}, \tag{5.2}$$

with the following instantaneous wave function

$$\psi(x,t) = \langle x|n_{\omega(t)}\rangle = \left(\frac{m\omega(t)}{\pi\hbar}\right)^{1/4} \frac{1}{(2^n n!)} \exp\left\{-\frac{m\omega(t)}{2\hbar}x^2\right\} H_n\left(\sqrt{\frac{m\omega(t)}{\hbar}}x\right), \tag{5.3}$$

where $H_n$ is the Hermit polynomial to the $n^{th}$ order. We introduce the annihilation operator $\hat{a}$ and creation operator $\hat{a}^\dagger$

$$\hat{a} = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{q} + \frac{i}{m\omega}\hat{p}\right); \tag{5.4}$$

$$\hat{a}^\dagger = \sqrt{\frac{m\omega}{2\hbar}}\left(\hat{q} - \frac{i}{m\omega}\hat{p}\right). \tag{5.5}$$

From equation (5.4) and (5.5), it is easy to express $\hat{p}$ and $\hat{q}$ as function of the ladder operators $\hat{a}$ and $\hat{a}^\dagger$. Hence an alternative expression for the Hamiltonian $\hat{H}_0(\omega(t))$ would be

$$\hat{H}_0(\omega(t)) = \hbar\omega(t)\left(\hat{a}_t^\dagger\hat{a}_t + \frac{1}{2}\right). \tag{5.6}$$

An important relation between the ladder operators and the instantaneous eigenstate is that $\hat{a}$ lower the eigenstate down by one level and $\hat{a}^\dagger$ lift it up by one level

through

$$\hat{a}|n\rangle = \sqrt{n+1}|n+1\rangle, \tag{5.7}$$

$$\hat{a}^\dagger|n\rangle = \sqrt{n}|n-1\rangle. \tag{5.8}$$

### 5.1.2 The control Hamiltonian $\hat{H}_1(\omega(t))$

The control Hamiltonian to achieve the fast-forward adiabatic process on the time evolution of a system is given by equation (3.18). Here explicitly for the 1-D harmonic oscillator, the time derivative of the Hamiltonian $\hat{H}_0(\omega(t))$ is $\partial_t \hat{H}_0(\omega(t)) = m\dot{\omega}\omega\hat{q}^2$ with $\hat{q}$ expressed as the ladder operators by

$$\hat{q} = \sqrt{\frac{\hbar}{2m\omega}}(\hat{a} + \hat{a}^\dagger). \tag{5.9}$$

To distinguish mass from the quantum number $m$, we use $M$ to represent mass in the following calculation. Hence the control Hamiltonian is calculated to be:

$$\begin{aligned}
\hat{H}_1(\omega(t)) &= i\hbar \sum_n \sum_{m\neq n} \frac{|m_{\omega(t)}\rangle\langle m_{\omega(t)}|\partial_t \hat{H}_0(\omega(t))|n_{\omega(t)}\rangle\langle n_{\omega(t)}|}{E_n(\omega(t)) - E_m(\omega(t))} \\
&= i\hbar \sum_n \sum_{m\neq n} \frac{|m_{\omega(t)}\rangle\langle m_{\omega(t)}|M\dot{\omega}\omega \left[\sqrt{\frac{\hbar}{2M\omega}}(\hat{a} + \hat{a}^\dagger)\right]^2 |n_{\omega(t)}\rangle\langle n_{\omega(t)}|}{\hbar\omega(n-m)} \\
&= \frac{i\hbar\dot{\omega}}{2\omega} \sum_n \sum_{m\neq n} \frac{|m_{\omega(t)}\rangle\langle m_{\omega(t)}|(\hat{a}^2 + \hat{a}^{\dagger 2} + \hat{a}\hat{a}^\dagger + \hat{a}^\dagger\hat{a})|n_{\omega(t)}\rangle\langle n_{\omega(t)}|}{n-m} \\
&= \frac{i\hbar\dot{\omega}}{2\omega} \sum_n \sum_{m\neq n} \frac{|m_{\omega(t)}\rangle\langle n_{\omega(t)}|}{n-m} (\sqrt{n(n-1)}\delta_{m,n-2} + \sqrt{(n+1)(n+2)}\delta_{m,n+2} \\
&\qquad + (n+1)\delta_{m,n} + n\delta_{m,n}) \\
&= \frac{i\hbar\dot{\omega}}{4\omega} \sum_n \left(\sqrt{n(n-1)}|(n-2)_{\omega(t)}\rangle\langle n_{\omega(t)}| - \sqrt{(n+1)(n+2)}|(n+2)_{\omega(t)}\rangle\langle n_{\omega(t)}|\right) \\
&= \frac{i\hbar\dot{\omega}}{4\omega} \sum_n (\hat{a}^2|n_{\omega(t)}\rangle\langle n_{\omega(t)}| - \hat{a}^{\dagger 2}|n_{\omega(t)}\rangle\langle n_{\omega(t)}|) \\
&= \frac{i\hbar\dot{\omega}}{4\omega}(\hat{a}^2 - \hat{a}^{\dagger 2}) \\
&= -\frac{\dot{\omega}}{4\omega}(\hat{q}\hat{p} + \hat{p}\hat{q}).
\end{aligned} \tag{5.10}$$

By adding the Hamiltonian $\hat{H}_1(\omega(t))$ specified by equation (5.10) to the original Hamiltonian $\hat{H}_0(\omega(t))$ with time dependent frequency $\omega(t)$, we realize the fast-forward adiabatic process on the 1-D quantum harmonic oscillator system.

### 5.1.3 The Thermal Ensemble

Same as in our study of two-level system, the initial state is prepared in the equilibrium thermal state at time $t = 0$ which forms a canonical ensemble

$$\rho(0) \equiv \frac{1}{Z_0} e^{-\beta \hat{H}_0(\omega(0))} = \sum_{n=0}^{\infty} \frac{e^{-\beta\hbar\omega_0(n+\frac{1}{2})}}{Z_0} |n_{\omega(0)}\rangle\langle n_{\omega(0)}|. \tag{5.11}$$

In the equation, $\omega_0$ is the angular frequency of the harmonic oscillator at time $t = 0$. Unlike the two-level system with only two energy levels, there are infinite energy levels in the harmonic oscillator system. Another important property is that the energy gap between adjacent levels is a constant value $\hbar\omega$. The partition function is thus

$$Z_0 \equiv Tr e^{-\beta \hat{H}_0(0)} = \sum_{n=0}^{\infty} e^{-\beta\hbar\omega_0(n+\frac{1}{2})} = \frac{e^{-\frac{1}{2}\beta\hbar\omega_0}}{1 - e^{-\beta\hbar\omega_0}}. \tag{5.12}$$

For an evolution from time 0 to $\tau$, the work function for non-adiabatic process is given by equation (2.8). With the existence of the control field $\hat{H}_1(t)$, there is no transitions between instantaneous eigenstates ($|n_{\omega(0)}\rangle \to |m_{\omega(\tau)}\rangle$ for $m \neq n$ is not allowed). Thus the work function is modified to

$$\begin{aligned} P(W) &= \sum_{n=0}^{\infty} P_n \delta \left( W - (E_n(\omega(\tau)) - E_n(\omega(0))) \right) \\ &= \sum_{n=0}^{\infty} e^{-n\beta\hbar\omega_0} (1 - e^{-\beta\hbar\omega_0}) \delta \left( W - \hbar(\omega_\tau - \omega_0)(n + \frac{1}{2}) \right). \end{aligned} \tag{5.13}$$

## 5.2 Numerical Simulation on 1-D Quantum Harmonic Oscillator

To study the convergence of Jarzynski equality in quantum harmonic oscillators, we set the control field $\hat{H}_1(\omega(t))$ to vanish at the beginning and end of the fast-forward process so that the work done to the system is still given by the same expression $W = E_m(\omega(\tau)) - E_n(\omega(0))$. This requires $\dot{\omega}(0) = \dot{\omega}(\tau) = 0$. An appropriate choice of $\omega(t)$ would be

$$\omega(t) = \omega_0 \sqrt{\frac{a^2+1}{2} - \frac{a^2-1}{2}\cos(n\pi\frac{t}{\tau})}. \tag{5.14}$$

with $\omega_0 = 10$, $a = \sqrt{3}$, $n = 1$, mass $m = 1$, evolution time $\tau = 10^{-4}$ and $\hbar = 1/2\pi$. It should be noticed that the parameters used in the simulation are dimensionless numbers. The final frequency $\omega(\tau)$ is greater than the initial frequency $\omega(0) = \omega_0$. Hence, in the fast-forward adiabatic process, the work done to the system would always be positive.

### 5.2.1 Transitions between Instantaneous Eigenstates

In non-adiabatic process, there are transitions between the instantaneous eigenstates during the evolution. It is essential for us to know the transition probabilities $p_{m|n}$ to investigate the work statistics of the process. To calculate $p_{m|n}$, we simulate the evolution of the eigenstate under $\hat{H}_0(\omega(t))$. The initial state is prepared in $|n_{\omega(0)}\rangle$ with $n = 1, 2, 3\cdots$ so that we obtain the information about the transitions when the evolving state starts with different eigenstates. The after-evolution wave function $\psi_n(x,\tau)$ is found using the split operator method. We use $\phi_m(x,\tau)$ to represent the wave function of instantaneous eigenstate $|m_{\omega(\tau)}\rangle$ of $\hat{H}_0(\omega(\tau))$. $\phi_m(x,\tau)$ could be calculated using equation (5.3). With the knowledge of both wave functions, the transition probability $p_{m|n}$ is simply given by the probability that the final state falls into eigenstate $|m_{\omega(\tau)}\rangle$ through

$$p_{m|n} = \left| \int dx \phi_m^*(x,\tau)\psi_n(x,\tau) \right|^2 \tag{5.15}$$

The process is repeated for $n = 0$ to 99 and $m = 0$ to 199 which is more than enough to ensure that we do not miss any trajectories with a reasonable probability. The table below shows the transition probability for the first few energy levels

TABLE 5.1: Transition probabilities for quantum harmonic oscillator with a time-dependent frequency

| states | $\|0_{\omega(\tau)}\rangle$ | $\|1_{\omega(\tau)}\rangle$ | $\|2_{\omega(\tau)}\rangle$ | $\|3_{\omega(\tau)}\rangle$ | $\|4_{\omega(\tau)}\rangle$ | $\|5_{\omega(\tau)}\rangle$ | $\|6_{\omega(\tau)}\rangle$ | $\cdots$ |
|---|---|---|---|---|---|---|---|---|
| $\|0_{\omega(0)}\rangle$ | 0.9634 | 0 | 0.0346 | 0 | 0.0019 | 0 | 0.0001 | $\cdots$ |
| $\|1_{\omega(0)}\rangle$ | 0 | 0.8943 | 0 | 0.0963 | 0 | 0.0086 | 0 | $\cdots$ |
| $\|2_{\omega(0)}\rangle$ | 0.0346 | 0 | 0.7671 | 0 | 0.1719 | 0 | 0.0235 | $\cdots$ |
| $\|3_{\omega(0)}\rangle$ | 0 | 0.0963 | 0 | 0.6020 | 0 | 0.2454 | 0 | $\cdots$ |
| $\|4_{\omega(0)}\rangle$ | 0.0019 | 0 | 0.1719 | 0 | 0.4242 | 0 | 0.3014 | $\cdots$ |
| $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\vdots$ | $\ddots$ |

More transition probabilities are in the table attached in Appendix B for reference. From Table 5.1, we again observe the transition symmetry for quantum harmonic oscillator as we do for two-level system. In deed, as long as the system undergoes unitary evolution, we will have this transition symmetry $p_{m|n} = p_{n|m}$. The proof goes as follows.

For any system undergoes unitary evolution during time interval $[0, \tau]$, we use $\hat{H}(\lambda(t))$ to represent the Hamiltonian and $|m_{\lambda(t)}\rangle$ to represent the instantaneous eigenstate of $\hat{H}(\lambda(t))$ at time $t$. The transition probability is given by

$$p_{m|n} = \langle m_{\lambda(\tau)}|\hat{U}|n_{\lambda(0)}\rangle\langle n_{\lambda(0)}|\hat{U}^\dagger|m_{\lambda(\tau)}\rangle; \tag{5.16}$$

$$p_{n|m} = \langle n_{\lambda(\tau)}|\hat{U}|m_{\lambda(0)}\rangle\langle m_{\lambda(0)}|\hat{U}^\dagger|n_{\lambda(\tau)}\rangle. \tag{5.17}$$

For unitary evolution, we can construct a transitionless driving so that $\hat{\tilde{U}}|n_{\lambda(0)}\rangle = e^{i\phi}|n_{\lambda(\tau)}\rangle$ where $\hat{\tilde{U}}$ is unitary and $\phi$ is the phase factor. Replace $|n_{\lambda(\tau)}\rangle$ with $e^{-i\phi}\hat{\tilde{U}}|n_{\lambda(0)}\rangle$ and we get

$$\begin{aligned} p_{m|n} &= \langle m_{\lambda(0)}|\hat{\tilde{U}}^\dagger e^{i\phi}\hat{U}|n_{\lambda(0)}\rangle\langle n_{\lambda(0)}|\hat{U}^\dagger e^{-i\phi}\hat{\tilde{U}}|m_{\lambda(0)}\rangle \\ &= \langle m_{\lambda(0)}|\hat{\tilde{U}}^\dagger\hat{U}|n_{\lambda(0)}\rangle\langle n_{\lambda(0)}|\hat{U}^\dagger\hat{\tilde{U}}|m_{\lambda(0)}\rangle; \end{aligned} \tag{5.18}$$

$$\begin{aligned} p_{n|m} &= \langle n_{\lambda(0)}|\hat{\tilde{U}}^\dagger e^{i\phi}\hat{U}|m_{\lambda(0)}\rangle\langle m_{\lambda(0)}|\hat{U}^\dagger e^{-i\phi}\hat{\tilde{U}}|n_{\lambda(0)}\rangle \\ &= \langle n_{\lambda(0)}|\hat{\tilde{U}}^\dagger\hat{U}|m_{\lambda(0)}\rangle\langle m_{\lambda(0)}|\hat{U}^\dagger\hat{\tilde{U}}|n_{\lambda(0)}\rangle. \end{aligned} \tag{5.19}$$

with $\hat{\tilde{U}}^\dagger \hat{U} \cdot \hat{U}^\dagger \hat{\tilde{U}} = \mathrm{I}$. So $A = \hat{\tilde{U}}^\dagger \hat{U}$ is unitary. Write $B = A|n_{\lambda(0)}\rangle\langle n_{\lambda(0)}|A^\dagger$, we obtain

$$p_{m|n} = \langle m_{\lambda(0)}|B|m_{\lambda(0)}\rangle \qquad p_{n|m} = \langle m_{\lambda(0)}|B^\dagger|m_{\lambda(0)}\rangle \tag{5.20}$$

Equation (5.20) and (5.21) implies that $p_{m|n} = p^*_{n|m}$. With $p_{m|n}$ and $p_{n|m}$ being real, the two equal each other. The transition symmetry hold for any unitary evolution. From this symmetry, we know that for an equilibrium thermal state $|\psi_i\rangle$ of an arbitrary system undergoing unitary time evolution, the adiabatic process gives the smallest possible expected work $\langle W_{ad}\rangle$. The proof goes as follows. Consider any unitary process and use $|\psi_f\rangle$ for final state in adiabatic process, $|\psi'_f\rangle$ for final state in other processes. And for simplicity, we use $P_n$ for the distribution of the initial thermal state, $\hat{H}_f$ for the Hamiltonian at the end of the process, and $E^f_n$ for the eigenenergy of $\hat{H}_f$.

$$\begin{aligned}
\langle W'\rangle - \langle W_{ad}\rangle &= \langle\psi'_f|\hat{H}_f|\psi'_f\rangle - \langle\psi_f|\hat{H}_f|\psi_f\rangle \\
&= \sum_m \sum_n P_n p_{m|n} E^f_m - \sum_n P_n E^f_n \\
&= \frac{1}{2}\sum_m \sum_n \left[(P_n p_{m|n} E^f_m + P_m p_{n|m} E^f_n) - (P_n p_{m|n} E^f_n + P_m p_{n|m} E^f_m)\right] \\
&= \frac{1}{2}\sum_m \sum_n p_{m|n}(P_n - P_m)(E^f_m - E^f_n).
\end{aligned} \tag{5.21}$$

When $E^f_m > E^f_n$, energy level $m$ is higher than energy level $n$, thus $P_n > P_m$. Hence, $\langle W'\rangle - \langle W_{ad}\rangle > 0$. When $E^f_m < E^f_n$, energy level $m$ is lower than energy level $n$, thus $P_n < P_m$. Hence, we also have $\langle W'\rangle - \langle W_{ad}\rangle > 0$. This implies the minimum limit of dissipated work $\langle W_{dis}\rangle = \langle W\rangle - \Delta F$ under unitary evolution is given by the dissipated work of an adiabatic process.

It is also noticed that eigenstate $|n_{\omega(0)}\rangle$ can only transit into eigenstate $|(n \pm 2m)_{\omega(\tau)}\rangle$ and is more likely to transit to higher energy level. Also, it is more likely to see a transition when the initial state is at a higher energy level. The selection of transition can be explained when we evaluate $\langle m_{\omega(t)}|\partial_t n_{\omega(t)}\rangle$ for our harmonic system. The other two observations are explained by Lutz in [22].

### 5.2.2 Convergence of Jarzynski Equality in 1-D Quantum Harmonic Oscillator

We simulate the convergence of Jarzynski equality under non-adiabatic and fast-forward adiabatic process at various temperatures to enhance our understanding on Jarzynski equality and to verify the efficiency of fast-forward adiabatic process in improving the convergence and the effect of temperature, negative works on the convergence. The procedure is the same as what we have done on two-level system. The initial state is prepared in equilibrium thermal state and an energy measurement is performed at $t = 0$. The state then evolves according to $\hat{H}_0(\omega(t))$ for non-adiabatic process and $\hat{H}(\omega(t)) = \hat{H}_0(\omega(t)) + \hat{H}_1(\omega(t))$ for fast-forward process respectively and another energy measurement is performed at the end of the process. With the process repeated, the averaged exponential work $\langle e^{-\beta W} \rangle$ is plotted against the number of trajectories. And when $\beta = 0.05$, the plot of the convergence of Jarzynski equality is shown in Figure 5.1.

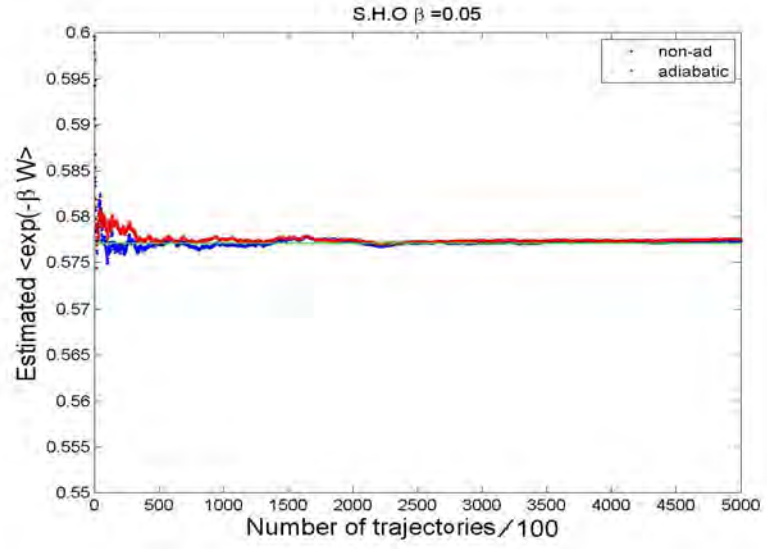


FIGURE 5.1: Simulation of the convergence of $\langle e^{-\beta W} \rangle$ for 1-D quantum harmonic oscillator at temperature $\beta = 0.05$. The blue dots represent the non-adiabatic process and the red ones represent the fast-forward adiabatic process. The green line is the theoretical value $e^{-\beta \Delta F} = 0.5770$ .

In Figure 5.1 and subsequent plots of the convergence of Jarzynski equality in our 1-D harmonic oscillator, we plot one dot for every 100 trajectories. At temperature $\beta = 0.05$, the converge speed under the two processes are the same. The idea of using fast-forward adiabatic process to accelerate the convergence of Jarzynski

equality does not work at high temperature on quantum harmonic oscillator, which is consistent with the result from two-level system.

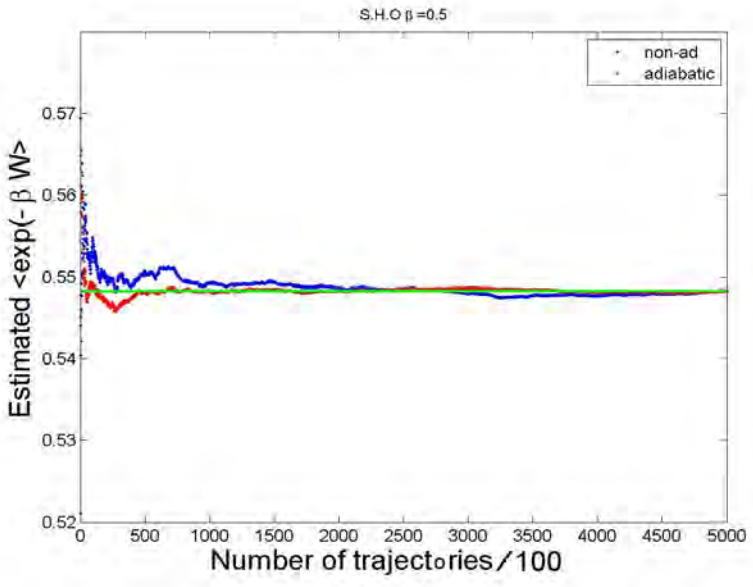


FIGURE 5.2: Simulation of the convergence of $\langle e^{-\beta W} \rangle$ for 1-D quantum harmonic oscillator at temperature $\beta = 0.5$. The blue dots represent the non-adiabatic process and the red ones represent the fast-forward adiabatic process. The green line is the theoretical value $e^{-\beta \Delta F} = 0.5483$ .

When the temperature is lowered to $\beta = 0.5$, the result from fast-forward adiabatic process begins to distinguish from that from non-adiabatic process as shown in Figure 5.2. Under adiabatic process, $\langle e^{-\beta W} \rangle$ converges to its expectation around the scale 500 while under non-adiabatic process, the convergence is done around scale 1000. When temperature decreases, the fast-forward process is more efficient in taking $\langle e^{-\beta W} \rangle$ to its expected value.

Just like what we did in the study of two-level system, the convergence of Jarzynski equality at different temperatures is also compared here. From plots in Figure 5.1 and 5.2, when temperature decreases from $\beta = 0.05$ to $\beta = 0.5$, the convergence for fast-forward adiabatic process is not greatly affected while for non-adiabatic process, it is significantly slowed down. The different effects of temperature on the two processes help to explain why fast-forward adiabatic process begins to surpass the non-adiabatic process on the converge speed when temperature decreases.

When temperature decreases further to $\beta = 1.5$, the improvement from fast-forward adiabatic process becomes larger as shown in Figure 5.3. Comparing Figure 5.3 and 5.2, with reduced temperature, we find that the convergence of

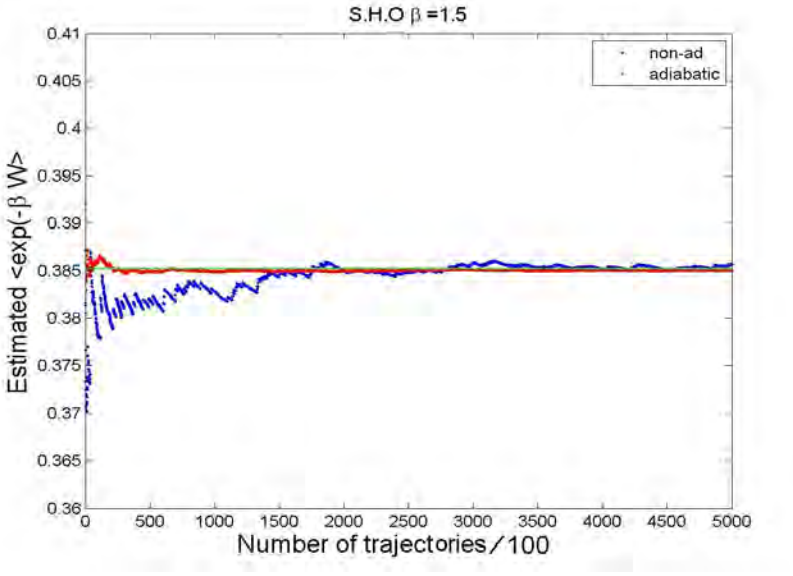


FIGURE 5.3: Simulation of the convergence of $\langle e^{-\beta W} \rangle$ for 1-D quantum harmonic oscillator at temperature $\beta = 1.5$. The blue dots represent the non-adiabatic process and the red ones represent the fast-forward adiabatic process. The green line is the theoretical value $e^{-\beta \Delta F} = 0.3852$ .

$\langle e^{-\beta W} \rangle$ under fast-forward adiabatic process becomes faster while for non-adiabatic process, the convergence speed continues to decrease. It is consistent with the situation in two-level system where the convergence is slightly slowed down and then speeded up for adiabatic process and always slowed down for non-adiabatic process with decreasing temperature.

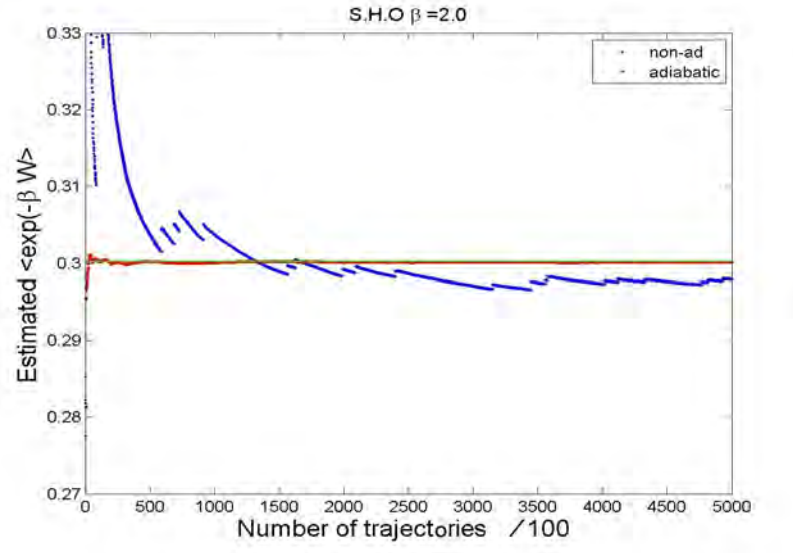


FIGURE 5.4: Simulation of the convergence of $\langle e^{-\beta W} \rangle$ for 1-D quantum harmonic oscillator at temperature $\beta = 2.0$. The blue dots represent the non-adiabatic process and the red ones represent the fast-forward adiabatic process. The green line is the theoretical value $e^{-\beta \Delta F} = 0.3002$ .

At $\beta = 2.0$, as shown in Figure 5.4, the improvement from fast-forward adiabatic process becomes very significant. In addition, we see jumps along the convergence path in the non-adiabatic case. These jumps are caused by the extreme values of $e^{-\beta W}$. When a negative work is realized, with a large value of $\beta$, the corresponding $e^{-\beta W}$ will be much greater than that with positive works. In the adiabatic process, transitions are suppressed. With the expression of work given by $W = (n + 1/2)\hbar(\omega(\tau) - \omega(0)$ and $\omega(\tau) > \omega(0)$, we do not have any negative work under adiabatic process for the harmonic oscillator system considered.

### 5.2.3 Analysis and Discussion

The simulation results on the convergence of Jarzynski equality in 1-D quantum harmonic oscillator shows that applying fast-forward adiabatic process does not affect the convergence at high temperature. When temperature decreases, the fast-forward adiabatic process comes into action and accelerates the convergence. The lower the temperature is, the larger the improvement we could achieve. The variance of $e^{-\beta W}$ and the dissipated work in table 5.2 shows the variance is almost the same for non-adiabatic and adiabatic process at high temperature and the difference between non-adiabatic and adiabatic process is getting larger when temperature decreases. Also, the adiabatic process has a smaller dissipated work.

TABLE 5.2: Variance of $e^{-\beta W}$ and Dissipated work $\langle W_{dis} \rangle$

| | | Variance $[\sigma^2(e^{-\beta W})]$ | Dissipated work $[\langle W_{dis} \rangle]$ |
|---|---|---|---|
| $\beta_1 = 0.05$ | Non-Adiabatic | 0.4473 | 8.9512 |
| | Adiabatic | 0.4057 | 3.6062 |
| $\beta_2 = 0.5$ | Non-Adiabatic | 0.4526 | 0.7508 |
| | Adiabatic | 0.3566 | 0.2817 |
| $\beta_3 = 1.5$ | Non-Adiabatic | 0.8730 | 0.3208 |
| | Adiabatic | 0.1506 | 0.0644 |
| $\beta_4 = 2.0$ | Non-Adiabatic | 1.6737 | 0.2629 |
| | Adiabatic | 0.0933 | 0.0312 |

The effect of temperature on non-adiabatic and adiabatic process is different. In the fast-forward adiabatic process, when temperature decreases, the variance of $e^{-\beta W}$ is getting smaller thus the convergence speed of $\langle e^{-\beta W} \rangle$ becomes faster. It is also noticed that the change of the convergence speed due to temperature change is not very large. In the non-adiabatic process, when temperature decreases, the variance grows, leading to a poorer convergence of Jarzynski equality. Compared

with the case in fast-forward adiabatic process, the temperature effect is contrary and is much more significant in the non-adiabatic process. Especially at a low temperature level, the decrease in temperature results in a big slow down on the convergence speed because of the negative work. At lower temperature, although the rate of having negative work for a trajectory gets smaller, once a negative work is observed, it produces an extreme value and greatly enlarges the variance of $e^{-\beta W}$. Those jumps in Figure 5.4 at $\beta = 2.0$ are evidence of the effect of negative work at low temperature. In general, the results from 1-D quantum harmonic oscillator are consistent with what we found in two-level system.

## 5.3 Degree of Adiabaticity and Convergence of Jarzynski Equality

The degree of adiabaticity measures how adiabatic a process is. For example, When the system experiences a fast-switch, we say the process is highly non-adiabatic; and when the system experiences a fast-forward adiabatic evolution, we say the system is strictly adiabatic. In this section, we study the relation between the degree of adiabaticity and the convergence of Jarzynksi equality.

We study on the same 1-D harmonic oscillator with time-dependent frequency described in the previous section of this chapter. The choice of $\omega(t)$ is again described by equation (5.14):

$$\omega(t) = \omega_0 \sqrt{\frac{a^2+1}{2} - \frac{a^2-1}{2}\cos(n\pi\frac{t}{\tau})},$$

with $\omega_0 = 10$, $a = \sqrt{3}$, mass $m = 1$, $\hbar = 1/2\pi$ and temperature $\beta = 1.5$. The evolution time $\tau$ is varied to achieve different degrees of adiabaticity. We use the quantity $\omega_0\tau$, which is the relative length of the evolution time $\tau$ to the natural period of the 1-D harmonic oscillator, as a measurement of the degree of adiabaticity of a process. We study the cases where $\tau = 0.01$, 0.1, 0.5, 1.0 with corresponding $\omega_0\tau = 0.1$, 1, 5, 10. It should be noticed that the quantity $\omega_0\tau$ only qualitatively measure the degree of adiabaticity. A larger $\omega_0\tau$ means a process is more adiabatic.

We use the same method as we do in subsection 5.2.2 to do the simulation of the convergence of Jarzynski equality and plot the convergence of $\langle e^{-\beta W}\rangle$ at $\beta = 1.5$

for the cases with $\omega_0\tau = 0.1,\ 1,\ 5,\ 10$. The plot for the convergence is shown in Figure 5.5.

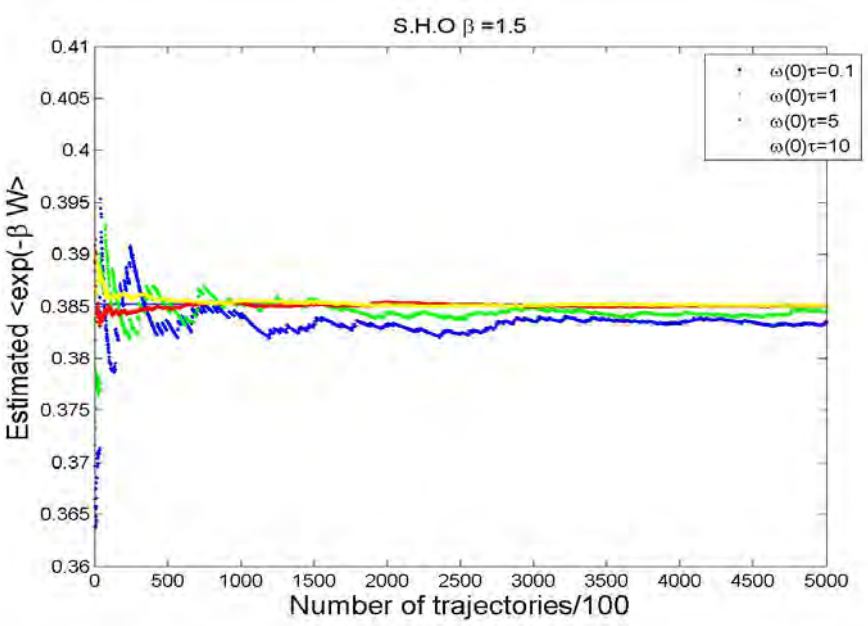


FIGURE 5.5: Convergence of $\langle e^{-\beta} \rangle$ in 1-D harmonic oscillator at $\beta = 1.5$ with various degree of adiabaticity. The blue dots are for the case when $\omega_0\tau = 0.1$; The green dots are for the case when $\omega_0\tau = 1$; The red dots are for the case when $\omega_0\tau = 5$ and The blue dots are for the case when $\omega_0\tau = 10$. The black line indicates the theoretical value $e^{-\beta\Delta F} = 0.3825$.

In Figure 5.5, it is easy to see that the averaged exponential work $\langle e^{-\beta W} \rangle$ with $\omega_0\tau = 5$ and $\omega_0\tau = 10$ (yellow line and red line respectively) converge to the expected value $e^{-\beta\Delta F}$ first. The convergence of $\langle e^{-\beta W} \rangle$ with $\omega_0\tau = 1$ (the green line) is slower and the convergence of $\langle e^{-\beta W} \rangle$ with $\omega_0\tau = 0.1$ (the blue line) is even slower. It shows that a larger value of $\omega_0\tau$ leads to a quicker convergence of $\langle e^{-\beta W} \rangle$; in other words, when a process becomes more adiabatic, the convergence of Jarzynski equality is accelerated. It should be noticed that this statement holds only when temperature is low. The explanation is the effect of negative works on the convergence discussed in subsection 5.2.3. When a process becomes more adiabatic, transitions between instantaneous eigenstates of the varying Hamiltonian are reduced, hence negative work realizations are also reduced; and at a low temperature, a reduction of negative works means a reduction of extreme values of $e^{-\beta W}$, hence a smaller variance of $e^{-\beta W}$ and hence a quicker convergence of Jarzynski equality.

# Chapter 6

# Conclusion

In this report, we discuss the impact on the convergence of Jarzynski equality when we use fast-adiabatic driving in the evolution of the system and study the effect of temperature, negative works on the convergence of Jaryznski equality and the relation between the degree of adiabaticity of a process and the convergence of Jarzynski equality.

We review Jarzynski equality and the adiabatic theorem. For Jarzynski equality, we explicitly show how the equation is derived in classical systems and quantum systems. For the adiabatic theorem, we review the conventional adiabatic approximation where the Hamiltonian must change very slowly and introduce transitionless quantum driving to achieve fast-forward adiabatic evolution. The restriction of slowly changing Hamiltonian is removed when we add an appropriate control field to the original time-dependent Hamiltonian.

The fast-forward adiabatic process is studied for a two-level system and 1-D quantum harmonic oscillator. For both systems, we study the transition probabilities and verify the transition symmetry and that the minimum limit of dissipated work $\langle W_{dis} \rangle = \langle W \rangle - \Delta F$ is given by an adiabatic process for an arbitrary system when the system undergoes unitary time evolution. We compare the convergence of Jarzynski equality under fast-forward adiabatic and non-adiabatic process for both systems at various temperatures and find that fast-forward process would accelerate the convergence of Jarzynski equality only at low temperatures. At high temperature, the two processes have the same result.

The effect of temperature and negative works on the convergence is discussed. The temperature affects the convergence in a different way for fast-forward process and non-adiabatic process. The convergence of Jarzynski equality under fast-forward adiabatic process is not largely affected by the change of temperature while under non-adiabatic process, the convergence is significantly slowed down when temperature decreases. As for negative works, they play an important role by producing extreme values of $e^{-\beta W}$ when temperature is low.

The relation between the degree of adiabaticity of a process and the convergence of Jarzynski equality is also studied. We compare the convergence of Jarzynski equality under processes with various degrees of adiabaticity at a low temperature and find that at low temperatures, when a process becomes more adiabatic, the convergence of Jarzynski equality is accelerated. This is consistent with the conclusion that fast-forward adiabatic process accelerates the convergence of Jarzynski equality at low temperatures.

The conclusion in this report is based on our study on a two-level system and 1-D quantum harmonic oscillator. However, we believe they hold in general as we study systems with both finite and infinite energy levels and more importantly, some fundamental elements in the argument will not change, and because of that feature, it is possible to suppress transitions between energy levels and hence negative works and hence accelerate the convergence. We emphasize that fast-forward adiabatic process eliminates transitions between instantaneous eigenstates of a fast-varying Hamiltonian and that at low temperature, negative works due to transition from high energy level to low energy level produce extreme value of $e^{-\beta W}$ hold in general.

# Appendix A

# The Convergence

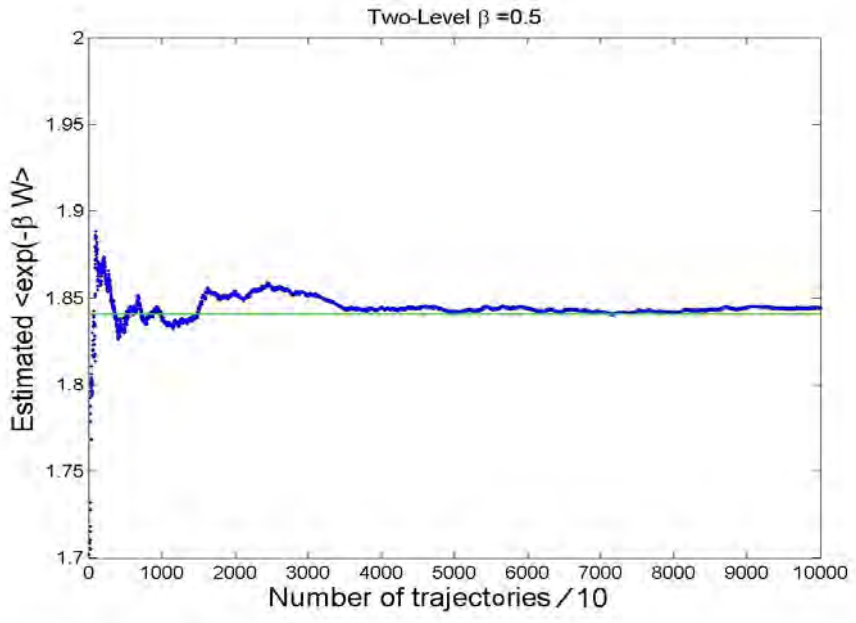


FIGURE A.1: Jarzynski convergence for two level system under non-adiabatic process at temperature $\beta = 0.5$

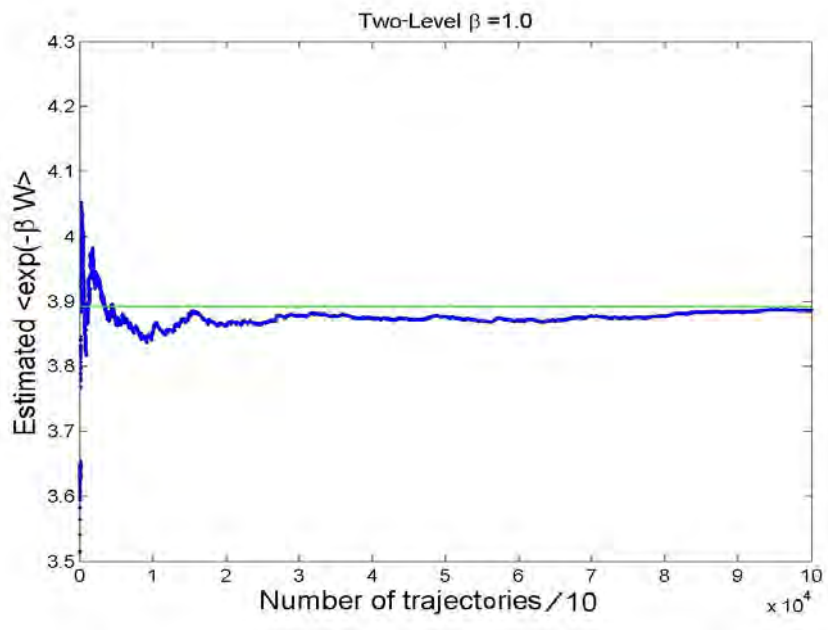


FIGURE A.2: Jarzynski convergence for two level system under non-adiabatic process at temperature $\beta = 1.0$

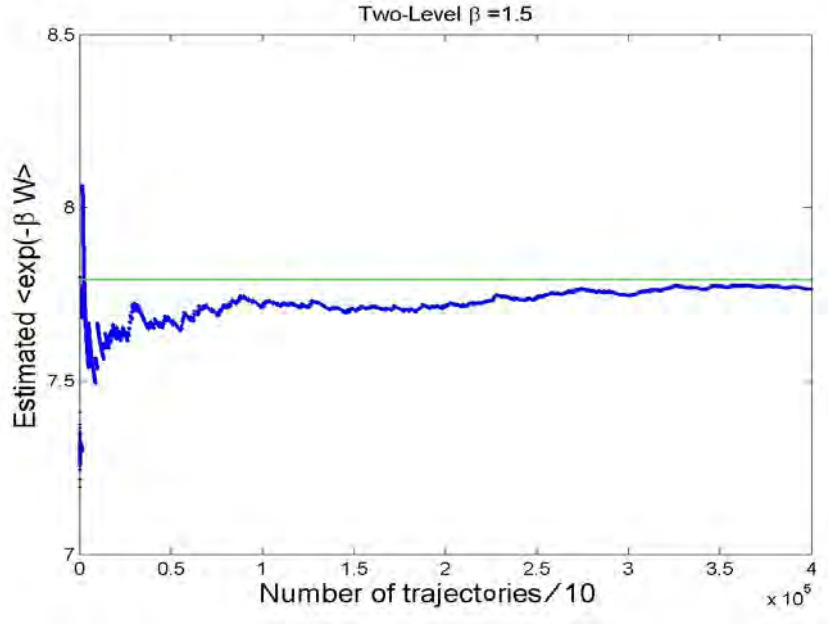


FIGURE A.3: Jarzynski convergence for two level system under non-adiabatic process at temperature $\beta = 1.5$

# Appendix B

# Transition Probabilities

TABLE B.1: Transition probabilities of 1-D harmonic oscillator with time-dependent frequency under non-adiabatic process

| | $\|1_{\omega(\tau)}\rangle$ | $\|2_{\omega(\tau)}\rangle$ | $\|3_{\omega(\tau)}\rangle$ | $\|4_{\omega(\tau)}\rangle$ | $\|5_{\omega(\tau)}\rangle$ | $\|6_{\omega(\tau)}\rangle$ | $\|7_{\omega(\tau)}\rangle$ | $\|8_{\omega(\tau)}\rangle$ |
|---|---|---|---|---|---|---|---|---|
| $\|1_{\omega(0)}\rangle$ | 0.9634 | 0 | 0.0346 | 0 | 0.0019 | 0 | 0.0001 | 0 |
| $\|2_{\omega(0)}\rangle$ | 0 | 0.8943 | 0 | 0.0963 | 0 | 0.0086 | 0 | 0.0007 |
| $\|3_{\omega(0)}\rangle$ | 0.0346 | 0 | 0.7671 | 0 | 0.1719 | 0 | 0.0235 | 0 |
| $\|4_{\omega(0)}\rangle$ | 0 | 0.0963 | 0 | 0.6020 | 0 | 0.2454 | 0 | 0.0482 |
| $\|5_{\omega(0)}\rangle$ | 0.0019 | 0 | 0.1719 | 0 | 0.4242 | 0 | 0.3014 | 0 |
| $\|6_{\omega(0)}\rangle$ | 0 | 0.0086 | 0 | 0.2454 | 0 | 0.2589 | 0 | 0.3286 |
| $\|7_{\omega(0)}\rangle$ | 0.0001 | 0 | 0.0235 | 0 | 0.3014 | 0 | 0.1267 | 0 |
| $\|8_{\omega(0)}\rangle$ | 0 | 0.0007 | 0 | 0.0482 | 0 | 0.3286 | 0 | 0.0403 |
| | $\|9_{\omega(\tau)}\rangle$ | $\|10_{\omega(\tau)}\rangle$ | $\|11_{\omega(\tau)}\rangle$ | $\|12_{\omega(\tau)}\rangle$ | $\|13_{\omega(\tau)}\rangle$ | $\|14_{\omega(\tau)}\rangle$ | $\|15_{\omega(\tau)}\rangle$ | $\|16_{\omega(\tau)}\rangle$ |
| $\|1_0\rangle$ | 0.0000 | 0 | 0.0000 | 0 | 0.0000 | 0 | 0.0000 | 0 |
| $\|2_0\rangle$ | 0 | 0.0000 | 0 | 0.0000 | 0 | 0.0000 | 0 | 0.0000 |
| $\|3_0\rangle$ | 0.0003 | 0 | 0.0000 | 0 | 0.0000 | 0 | 0.0000 | 0 |
| $\|4_0\rangle$ | 0 | 0.0009 | 0 | 0.0001 | 0 | 0.0000 | 0 | 0.0000 |
| $\|5_0\rangle$ | 0.0154 | 0 | 0.0023 | 0 | 0.0003 | 0 | 0.0000 | 0 |
| $\|6_0\rangle$ | 0 | 0.0290 | 0 | 0.0053 | 0 | 0.0008 | 0 | 0.0001 |
| $\|7_0\rangle$ | 0.1650 | 0 | 0.0485 | 0 | 0.0106 | 0 | 0.0019 | 0 |
| $\|8_0\rangle$ | 0 | 0.2010 | 0 | 0.0735 | 0 | 0.0190 | 0 | 0.0039 |

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