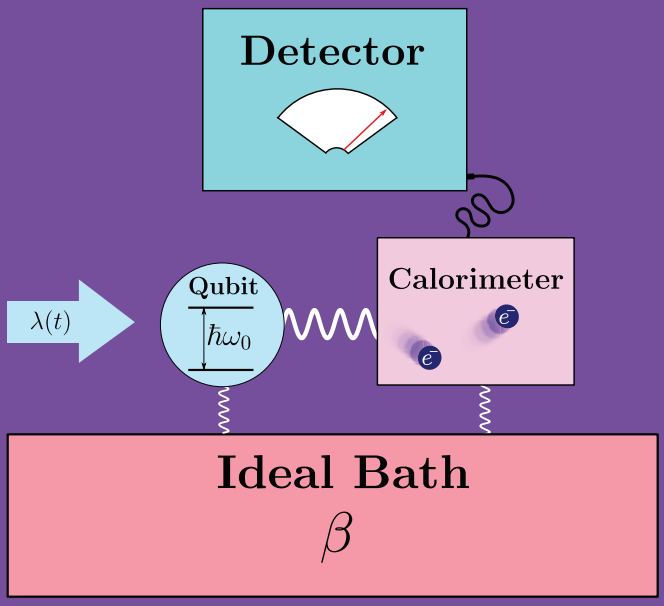
Department of Applied Physics

Work statistics in open quantum systems

Samu Suomela



Aalto University

DOCTORAL DISSERTATIONS

Aalto University publication series
DOCTORAL DISSERTATIONS 15/2017

Work statistics in open quantum systems

Samu Suomela

A doctoral dissertation completed for the degree of Doctor of Science (Technology) to be defended, with the permission of the Aalto University School of Science, at a public examination held at the lecture hall M1 (Otakaari 1, Espoo) of the school on 13th of February 2017 at 2 pm.

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Aalto University publication series
DOCTORAL DISSERTATIONS 15/2017

ISBN 978-952-60-7264-7 (printed)
ISBN 978-952-60-7263-0 (pdf)
ISSN-L 1799-4934
ISSN 1799-4934 (printed)
ISSN 1799-4942 (pdf)
http://urn.fi/URN:ISBN:978-952-60-7263-0

Unigrafia Oy
Helsinki 2017

Finland

441 697
Printed matter

Aalto University

Abstract

Aalto University, P.O. Box 11000, FI-00076 Aalto www.aalto.fi

Author
Samu Suomela

Name of the doctoral dissertation
Work statistics in open quantum systems

Publisher School of Science

Unit Department of Applied Physics

Series Aalto University publication series DOCTORAL DISSERTATIONS 15/2017

Field of research Theoretical and Computational Physics

Manuscript submitted 11 November 2016 **Date of the defence** 13 February 2017

Permission to publish granted (date) 11 January 2017 **Language** English

☐ **Monograph** ☒ **Article dissertation** ☐ **Essay dissertation**

Abstract

Rapid progress in the fabrication and manipulation of micro and nanoscale devices has made it necessary to extend the concepts of thermodynamics to small systems and finally to quantum systems. In such systems the extensive thermodynamic quantities, such as entropy, heat, and work, are not described by their average values alone but by distributions.

Remarkably, it has been shown that the stochastic thermodynamic variables often obey fluctuation relations which usually appear in the form of relations between exponential averages. While the two-measurement protocol of thermodynamic variables, especially work, is now well studied in closed quantum systems, there have been conceptual and experimental problems in open quantum systems.

In this thesis, we theoretically study work statistics and fluctuation relations in open quantum systems. To calculate the work statistics, we use the quantum jump method and direct master equation calculations. We show that work definitions equivalent in closed systems can lead to mutually different results in the case of open quantum systems due to a different order of approximations. Moreover, we show that the fluctuation relations can be extended to nearly adiabatically driven systems by using the adiabatic renormalization procedure.

Last, we focus on how a finite size of the environment affects the dynamics and work statistics of open quantum systems. This is important from the experimental point of view because a finite-size environment allows the detection of heat exchange between the system and the environment. We derive a master equation that takes into account these effects and develop a stochastic model that unravels the master equation. We explicitly show that the finite size of the environment influences the dynamics and the work statistics. We also show that the common fluctuation relations are still valid.

Keywords open quantum systems, work fluctuations, stochastic thermodynamics, quantum jump method, finite environment

ISBN (printed) 978-952-60-7264-7 **ISBN (pdf)** 978-952-60-7263-0

ISSN-L 1799-4934 **ISSN (printed)** 1799-4934 **ISSN (pdf)** 1799-4942

Location of publisher Helsinki **Location of printing** Helsinki **Year** 2017

Pages 111 **urn** http://urn.fi/URN:ISBN:978-952-60-7263-0

A? Aalto-yliopisto

Tiivistelmä

Aalto-yliopisto, PL 11000, 00076 Aalto www.aalto.fi

Tekijä
Samu Suomela

Väitöskirjan nimi
Työn statistiikka avoimissa kvanttimekaanisissa systeemeissä.

Julkaisija Perustieteiden korkeakoulu

Yksikkö Teknillisen fysiikan laitos

Sarja Aalto University publication series DOCTORAL DISSERTATIONS 15/2017

Tutkimusala Teoreettinen ja laskennallinen fysiikka

Käsikirjoituksen pvm 11.11.2016 **Väitöspäivä** 13.02.2017

Julkaisuluvan myöntämispäivä 11.01.2017 **Kieli** Englanti

☐ **Monografia** ☒ **Artikkeliväitöskirja** ☐ **Esseeväitöskirja**

Tiivistelmä

Nopea kehitys pienten komponenttien valmistamisessa on tehnyt tarpeelliseksi laajentaa termodynamiikan konseptit pieniin systeemeihin ja lopulta kvanttimekaanisiin systeemeihin. Näiden systeemien pienen koon takia termodynaamisia suureita, kuten työtä ja lämpöä, ei voida kuvata pelkällä keskiarvolla, vaan koko jakauma täytyy ottaa huomioon.

Tässä väitöskirjassa tutkitaan työn statistiikkaa avoimissa kvanttisysteemeissä. Väitöskirjassa näytetään, että työn määritelmät, jotka ovat yhtenevät suljetuille systeemeille, voivat johtaa eri tuloksiin avoimissa kvanttisysteemeissä. Työssä laajennetaan myös työn fluktuaatiorelaatiot lähes adiabaattisesti ajasta riippuviin systeemeihin.

Väitöskirjassa kehitetään myös malli, joka ottaa huomioon ympäristön äärellisen koon. Tämä malli mahdollistaa työn mittaamiseen ehdotettujen kokeiden mallintamisen, joissa ympäristön koon täytyy olla pieni lämmönvaihdon mittaamiseksi. Mallille kehitetään myös stokastinen vastine, joka mahdollistaa stokastisen termodynaamikan käytön työn ja lämmön analysoimiseen.

Väitöskirjassa kehitetyt menetelmät mahdollistavat termodynamiikan tutkimisen systeemeissä, joita ei tavanomaisilla menetelmillä pystytä tutkimaan.

Avainsanat avoimet kvanttisysteemit, termodynamiikka, stokastinen termodynamiikka, työfluktuaatiot

ISBN (painettu) 978-952-60-7264-7 **ISBN (pdf)** 978-952-60-7263-0

ISSN-L 1799-4934 **ISSN (painettu)** 1799-4934 **ISSN (pdf)** 1799-4942

Julkaisupaikka Helsinki **Painopaikka** Helsinki **Vuosi** 2017

Sivumäärä 111 **urn** http://urn.fi/URN:ISBN:978-952-60-7263-0

Preface

The work presented in this dissertation was carried out in the Multiscale Statistical Physics (MSP) group at the Department of Applied Physics, Aalto University during years 2013-2016. The work has been supported by the Vilho, Kalle and Yrjö Väisälä Foundation and the Center of Excellence in Computational Nanoscience (COMP).

First of all, I would like to thank my supervisor Prof. Tapio Ala-Nissilä. I have worked with Tapio since 2010. First, as a summer student and finally as a PhD student. Under Tapio's guidance, I have learned what I know about scientific research. I am especially grateful to the working environment created by Tapio and the opportunity to influence the direction of my research.

Secondly, I would like to thank Prof. Jukka Pekola, whose infectious enthusiasm for physics and hands-on attitude towards scientific questions have been influential for my PhD work. I would also like to thank my other collaborators outside of MSP group, especially Prof. Joachim Ankerhold, Dr. Mikko Möttönen, Dr. Juha Salmilehto and Dr. Paolo Solinas. I have enjoyed our conversations and this thesis would not be the same without your impact.

I also had the pleasure to work with the fellow MSP group members, Dr. Aki Kutvonen, Dr. Ivan Savenko, M.Sc. Rui Sampaio and Dr. Rebecca Schmidt. Our frequent conversations related and unrelated to physics, have been helpful for completing the work presented in this thesis.

I would also like to express my appreciation to the other past and present group members, e.g., Dr. Vaibhav Thakore, Dr. Jalal Sarabadani, M.Sc. Michiko Alcanzare, Dr. Santtu Ollila, Dr. Harri Mökkönen, Dr. Vili Heinonen, Dr. Cristian Achim and M.Sc. Petri Hirvonen. Although,

we have not worked that much together, I have always felt camaraderie amongst you. I have enjoyed our trips together both abroad and in Finland.

I would also like to thank the other people on the corridor, such as Dr. Miguel Caro, Dr. Leonardo Espinosa, M.Sc. Jouko Lehtomäki, Dr. Jingrui Li, Dr. Tiziana Musso, M.Sc. Tuomas Rossi and Dr. Azier Zugarramurdi to name of a few. Many of you I can call as dear friends. I have enjoyed our tea breaks and other activities. I would also like to express my gratitude to all the participants of the department's floorball sessions. I had a lot of fun. Thanks also to Eija Järvinen for taking care of the travel arrangements and bringing some common sense to the corridor.

I would also like to thank my family and friends. Thank you, mum and dad for creating such a lovely environment to grew up in. Thank you for supporting and inspiring me. Without my dad, who past away during my PhD studies, I might not have gotten interested in science, let alone do a PhD. Also my sisters, Hanne and Erika, I could not have hoped for better elder sisters. Of course, thank you to my nephew and nieces, Eevi, Eetu, Sina and Saana. Looking at you, makes me appreciate what really matters in life.

Last, I want to thank you, Shilpi, my love. Thank you for all the great moments we have had and will have. There is so many things about you that I'm thankful. Thank you for being by my side.

Espoo, January 17, 2017,

Samu Suomela

Contents

List of Publications

This thesis consists of an overview and of the following publications which are referred to in the text by their Roman numerals.

I S. Suomela, P. Solinas, J. P. Pekola, J. Ankerhold, T. Ala-Nissilä. Moments of work in the two-point measurement protocol for a driven open quantum system. *Physical Review B*, Volume 90, Issue 9, 094304 (8 pages), September 2014.

II S. Suomela, J. Salmilehto, I. G. Savenko, T. Ala-Nissilä, and M. Möttönen. Fluctuations of work in a nearly adiabatically driven open quantum system. *Physical Review E*, Volume 91, Issue 2, 022126 (13 pages), January 2015.

III S. Suomela, A. Kutvonen and T. Ala-Nissilä. Quantum jump model for a system with a finite-size environment. *Physical Review E*, Volume 93, Issue 6, 062106 (7 pages), June 2016.

IV S. Suomela, R. Sampaio and T. Ala-Nissilä. Comparison between quantum jumps and master equation in the presence of a finite environment. *Physical Review E*, Volume 94, Issue 4, 032138 (9 pages), September 2016.

Author's Contribution

Publication I: "Moments of work in the two-point measurement protocol for a driven open quantum system"

The author derived the analytical results and did most of the numerical calculations. The author wrote the first version of the manuscript.

Publication II: "Fluctuations of work in a nearly adiabatically driven open quantum system"

The author did the numerical calculations and derived most of the analytical results. The author wrote the first versions of the introduction, the methods and the results sections.

Publication III: "Quantum jump model for a system with a finite-size environment"

The author did the numerical calculations and derived the analytical results. The author wrote the first version of the manuscript.

Publication IV: "Comparison between quantum jumps and master equation in the presence of a finite environment"

The author derived the analytical results and did most of the numerical calculations. The author wrote the first version of the manuscript.

During his doctoral studies, the author has also contributed to the related articles [1–5], excluded from this thesis.

1. Introduction

Thermodynamics has been one of the most triumphant theories of the last millennium, explaining a variety of scientific and engineering problems encountered with macroscopic systems. The standard theory of equilibrium thermodynamics focuses on large ensembles described solely by a few average quantities, which appear in the laws of thermodynamics and equations of state [6]. This remarkable simplification can be microscopically explained by using a statistical description known as statistical mechanics.

The fast progress made in the fabrication of micro and nanoscale devices [7–10] has made it desirable to extend the tools of thermodynamics to small-scale systems and finally to the quantum realm. However, such small systems are usually easily driven away from equilibrium and thus cannot be described with the standard equilibrium thermodynamics or statistical mechanics. For these systems, it is not enough to simply use averages of thermodynamic quantities such as internal energy, work, heat and entropy. Even near equilibrium, the fluctuations must be taken into account as the relative fluctuations scale $\propto N^{-1/2}$ with the number of degrees of freedom N. When a process occurs near equilibrium, the deviation from equilibrium can be treated perturbatively using linear response theories [11–13]. However, these theories still rely on equilibrium ensembles and therefore cannot be applied far from equilibrium.

In the past few decades, fluctuation relations [14–17] have opened a new way to tackle the obscure nature of nonequilibrium processes even far from equilibrium. These relations form equalities between exponentiated thermodynamic quantities instead of usual inequalities occurring in thermodynamics. Perhaps the most well-known of these is the Jarzyn-

ski equality [15] derived in 1997 that connects the average exponentiated work performed on a driven system with the free-energy difference between the initial and final thermal distributions. The study of fluctuation relations, however, has a longer history dating back to the works of Zwanzig [18], Bochkov and Kuzovlev [14], and to the study of steady state entropy production by Yamada and Kawasaki [19], Evans et al. [20, 21], and Gallavotti and Cohen [22].

For classical systems the relevant fluctuation relations have been verified in multiple occasions [23–28]. However, for quantum mechanical systems, the situation is more problematic. Due to the obscure behavior of quantum systems such as superposition and entanglement, it has been far from trivial how to extend thermodynamic quantities and fluctuation relations into the quantum regime. For example, the definition of work has caused much debate [29–32]. Only recently using a two point measurement definition of work [31, 33–35], the Jarzynski equality has been shown to hold within the experimental accuracy for closed quantum systems[1] [36, 37]. However, a closed system is always an idealization. In real life, the system always interacts with its surroundings. These kind of quantum systems are called *open quantum systems*.

A common approach to extend the fluctuation relations into open quantum systems involves an assumption of weak coupling between the system and the environment [31, 35]. Additionally, in order to compute the work statistics and fluctuation relations, an infinitely large or memoryless environment is usually assumed [35, 38–41].

In this thesis, we study work statistics and fluctuation relations in weakly coupled open quantum systems. We start by briefly introducing the master equation formalism of open quantum systems in Chapter 2. We also show how the Lindblad master equation can be unravelled into stochastic trajectories with the quantum jump method. These trajectories offer a natural way to study thermodynamics in open quantum systems as they try to mimic the individual realizations in experiments. In Chapter 3, we focus on the different definitions of work and how the fluctuation relations can be derived for open quantum systems. We also show how to calculate the thermodynamic quantities, such as work and entropy, for stochastic

[1] We use the term 'closed system' to denote a system completely isolated from its surroundings.

trajectories by using the concepts of stochastic thermodynamics [42].

In Chapter 4, we focus on a specific open quantum system that is weakly and sinusoidally driven by a classical source. The environment is assumed to be infinitely large such that the Lindbad equation can be used. We show that the Jarzynski equality is valid for such system and that the two point measurement definition of work agrees with the power operator approach [43] if the driving is in resonance. However, for off-resonance driving, the results deviate from each other. This chapter summarizes Publication I with some results taken from Publication IV.

In Chapter 5, we study a similar system but with a strong and slow driving. As the driving is slow, we use the adiabatic renormalization procedure to accurately take into account the effect of driving[2]. We show that the common fluctuation relations hold when the definition of work and the dynamics follow the same order of renormalization procedure. This chapter summarizes Publication II.

The above chapters deal with an infinitely large environment. In Chapter 6, we focus on dynamics and thermodynamics in the presence of a finite but large environment. We derive a master equation for the setup and develop a finite environment quantum jump model that unravels the master equation. We show that due to the finite-size of the environment, the trajectories depend on their own history and thus can be thought as non-Markovian. As the total system is again closed, the common fluctuation relations are shown to hold, given that the necessary conditions are fulfilled. This chapter summarizes Publications III and IV.

Finally, Chapter 7 concludes the results presented in this thesis and presents possible future direction for the research.

[2]For arbitrary driving speed, Floquet theory can be used to describe the dynamics and work statistics [44–46] if the drive is periodic.

2. Open quantum systems

The time evolution of an open quantum system is conventionally described by an effective equation of motion called the master equation. In this chapter, we present the microscopic derivation of the Lindblad master equation, which is currently the most widely used master equation in quantum physics. We also introduce the quantum jump method that unravels the Lindblad equation into stochastic trajectories.

2.1 Liouville-von Neumann equation

In quantum mechanics, the time evolution of a closed system is postulated to follow the Schrödinger equation. In the density matrix formalism, this equation is known as the Liouville–von Neumann equation and it can be expressed as

$$\dot{\hat{\rho}}(t) = -\frac{i}{\hbar}\left[\hat{H}(t), \hat{\rho}(t)\right], \tag{2.1}$$

where $\hat{\rho}$ and $\hat{H}$ are the density matrix and the Hamiltonian of the system, respectively. However, a real system can never be completely isolated from its environment. If the interaction with the environment affects the system's evolution, the quantum system is called *open* and it's evolution doesn't obey Eq. (2.1). Nevertheless, Eq. (2.1) still offers a convenient starting point to describe the system dynamics as the system-environment composite can be approximated as a closed system.

2.2 Microscopic derivation of Markovian quantum master equation

Let us start the discussion with the total Hamiltonian of the system-environment composite. Following the standard treatment [47], the total Hamiltonian can be separated into three parts:

$$\hat{H}_{\mathrm{Tot}}(t) = \hat{H}_S(t) + \hat{V} + \hat{H}_E, \tag{2.2}$$

where $\hat{H}_S$ depends only on the system degrees of freedom and is defined as the system Hamiltonian. The operator $\hat{V}$ is the system-environment coupling operator that depends on both the system and environment degrees of freedom. The last term $\hat{H}_E$ depends on the environment degrees of freedom and is defined as the Hamiltonian of the environment.

We assume the composite system to be closed. Consequently, its time-evolution is given by Eq. (2.1). By changing into the interaction picture with respect to $\hat{H}_S(t) + \hat{H}_E$, the time evolution of the total density matrix $\hat{\rho}_I$ is given by

$$\dot{\hat{\rho}}_I(t) = -\frac{i}{\hbar}\left[\hat{V}_I(t), \hat{\rho}_I(t)\right]. \tag{2.3}$$

where we use the subscript I to denote the interaction picture, e.g. $\hat{V}_I(t) = \hat{U}_{SE}^{\dagger}(t)\hat{V}\hat{U}_{SE}(t)$ with time evolution operator $\hat{U}_{SE}(t) = \mathcal{T}_{\leftarrow} e^{-\frac{i}{\hbar}\int_0^t \left[\hat{H}_S(t') + \hat{H}_E\right] dt'}$. Here, $\mathcal{T}_{\leftarrow}$ denotes the chronological time-ordering. By integrating Eq. (2.3) and inserting the result to the right side of Eq. (2.3), leads to

$$\dot{\hat{\rho}}_I(t) = -\frac{i}{\hbar}\left[\hat{V}_I(t), \hat{\rho}_I(0)\right] - \frac{1}{\hbar^2}\int_0^t \left[\hat{V}_I(t), \left[\hat{V}_I(t'), \hat{\rho}_I(t')\right]\right] dt'. \tag{2.4}$$

The master equation for the system density matrix is obtained by tracing over the environment degrees of freedom:

$$\dot{\hat{\rho}}_{S,I}(t) = -\frac{i}{\hbar}\mathrm{Tr}_E\left\{\left[\hat{V}_I(t), \hat{\rho}_I(0)\right]\right\} - \frac{1}{\hbar^2}\int_0^t \mathrm{Tr}_E\left\{\left[\hat{V}_I(t), \left[\hat{V}_I(t'), \hat{\rho}_I(t')\right]\right]\right\} dt', \tag{2.5}$$

where $\hat{\rho}_{S,I}(t) = \mathrm{Tr}_E\{\hat{\rho}_I(t)\}$. Up to this point, there are no approximations. However, the presence of the total density matrix on the right hand side of Eq. (2.5) makes it difficult to use.

In order to simplify the expression, we assume the coupling between the system and the environment to be weak. This allows us to treat the coupling perturbatively. We can eliminate $\hat{\rho}_I(t)$ from Eq. (2.5) with an approximation called the *Born approximation* [47], which assumes that the coupling is so weak that the influence on the environment is minimal:

$$\hat{\rho}_I(t) \approx \hat{\rho}_{S,I}(t) \otimes \hat{\rho}_E(0). \tag{2.6}$$

We also assume the coupling operator $\hat{V}_I$ and the initial state $\hat{\rho}_I(0) = \hat{\rho}_S(0) \otimes \hat{\rho}_E(0)$ are such that $\mathrm{Tr}_E \left\{ \left[\hat{V}_I(t), \hat{\rho}_I(0) \right] \right\} = 0$. With these assumptions, the master equation simplifies to

$$\dot{\hat{\rho}}_{S,I}(t) = -\frac{1}{\hbar^2} \int_0^t \mathrm{Tr}_E \left\{ \left[\hat{V}_I(t), \left[\hat{V}_I(t'), \hat{\rho}_{S,I}(t') \otimes \hat{\rho}_E(0) \right] \right] \right\} dt'. \tag{2.7}$$

Equation (2.7), however, is not *Markovian* as the integrand contains $\hat{\rho}_{S,I}(t')$ and thus the evolution of $\hat{\rho}_S(t)$ depends on its history. The equation can be made $Markovian$ by replacing the integral's upper limit with ∞ and by replacing $\hat{\rho}_{S,I}(t')$ with $\hat{\rho}_{S,I}(t)$ in the integrand. This is justified if the changes in system are much slower than the decay of environment correlation functions [48]. With these approximations, we obtain the Markovian master equation [47]:

$$\dot{\hat{\rho}}_{S,I}(t) = -\frac{1}{\hbar^2} \int_0^\infty \mathrm{Tr}_E \left\{ \left[\hat{V}_I(t), \left[\hat{V}_I(t'), \hat{\rho}_{S,I}(t) \otimes \hat{\rho}_E(0) \right] \right] \right\} dt'. \tag{2.8}$$

2.3 Lindblad equation

Although Eq. (2.8) is Markovian, it is not enough to guarantee the positivity of the system density matrix $\hat{\rho}_{S,I}(t)$. As shown by G. Lindblad in 1976[1] [49], the most general form of a Markovian master equation that preserves the trace and the positivity of the system density matrix is given by

$$\dot{\hat{\rho}}_S(t) = -\frac{i}{\hbar} \left[\hat{H}_{\text{eff}}(t), \hat{\rho}_S(t) \right] + \sum_j \Gamma_j \left(\hat{L}_j \hat{\rho}_S(t) \hat{L}_j^\dagger - \frac{1}{2} \left\{ \hat{L}_j^\dagger \hat{L}_j, \hat{\rho}_S(t) \right\} \right), \tag{2.9}$$

where $\hat{H}_{\text{eff}}(t)$ is the effective system Hamiltonian, $\hat{L}_j$ are known as Lindblad operators and the transition rates Γ_j are non-negative. This equation is known as the *Lindblad equation*. The Markovian master equation of Eq. (2.8) can be casted to the celebrated Lindblad form by an additional approximation known as the secular approximation [47, 48], which neglects the fast oscillating coupling terms.

[1] In the proof, $\hat{H}_{\text{eff}}$ and $\hat{L}_j$ are assumed to be bounded.

2.4 Quantum jump method

Instead of directly evolving the density matrix according to the Lindblad equation [Eq. (2.9)], the dynamics of the open system can also be obtained with a stochastic method, known as the quantum jump method[2] [50–52]. The quantum jump method unravels the system's evolution into stochastic trajectories with environment induced jumps. When averaging over all the trajectories, the quantum jump method has been shown to produce the same density matrix evolution as the corresponding Lindblad equation [51], which can also be expressed in the form

$$\dot{\hat{\rho}}_S(t) = -\frac{i}{\hbar}\left[\hat{H}_{\text{eff}}(t), \hat{\rho}_S(t)\right] - \frac{1}{2}\sum_j \left\{\hat{C}_j^\dagger \hat{C}_j, \hat{\rho}_S(t)\right\} + \sum_j \hat{C}_j \hat{\rho}_S(t) \hat{C}_j^\dagger, \quad (2.10)$$

where $\hat{C}_j = \sqrt{\Gamma_j}\hat{L}_j$ are known as *jump operators*. When described with the quantum jump method, the first two terms on the right-hand side of Eq. (2.10) are given by no-jump evolution and the last term is caused by stochastic jumps.

Let us now introduce briefly the protocol of the quantum jump method. For each time step, the protocol can be divided into two parts [51]:

Step 1:

Consider an open quantum system coupled to an environment with jump operators $\hat{C}_j$. Let us define a non-hermitian Hamiltonian $\hat{H}$ such that

$$\hat{H}(t) = \hat{H}_{\text{eff}}(t) - \frac{i\hbar}{2}\sum_j \hat{C}_j^\dagger \hat{C}_j. \quad (2.11)$$

Suppose that the system is in a state $|\phi(t)\rangle$ at time t. We can form a new state $|\phi^{(1)}(t+\delta t)\rangle$ by evolving the state $|\phi^{(1)}(t)\rangle$ with the non-hermitian Hamiltonian $\hat{H}$. For a very small time step δt, the state $|\phi^{(1)}(t+\delta t)\rangle$ can be approximated by

$$|\phi^{(1)}(t+\delta t)\rangle \approx e^{-\frac{i}{\hbar}\hat{H}(t)\delta t}|\phi(t)\rangle \approx \left(1 - \frac{i}{\hbar}\hat{H}(t)\delta t\right)|\phi(t)\rangle. \quad (2.12)$$

As $\hat{H}$ is non-hermitian, the norm of $|\phi^{(1)}(t+\delta t)\rangle$ deviates slightly from unity:

$$\langle\phi^{(1)}(t+\delta t)|\phi^{(1)}(t+\delta t)\rangle \approx 1 - \delta p, \quad (2.13)$$

where up to the first order of δt, $\delta p = \sum_j \delta p_j$ with $\delta p_j = \delta t \langle\phi(t)|\hat{C}_j^\dagger \hat{C}_j|\phi(t)\rangle$.

[2] Also known in the literature as the Monte Carlo wave function method.

Step 2:

Let us generate a uniformly distributed pseudorandom number $\epsilon \in [0, 1]$. If $\epsilon > \delta p$, no jump occurs and the new normalized state at $t + \delta t$ is given by

$$|\phi(t + \delta t)\rangle = \frac{|\phi^{(1)}(t + \delta t)\rangle}{\sqrt{1 - \delta p}}. \tag{2.14}$$

However, if $\epsilon < \delta p$, a quantum jump occurs. The new normalized state is chosen from the different states $\hat{C}_j|\phi(t)\rangle$ according to the probability $\delta p_j/\delta p$:

$$|\phi(t + \delta t)\rangle = \frac{\hat{C}_j|\phi(t)\rangle}{\sqrt{\delta p_j/\delta t}}. \tag{2.15}$$

After the new wave function $|\phi(t + \delta t)\rangle$ has been formed, the procedure is repeated for $|\phi(t + \delta t)\rangle$ starting from step 1.

3. Quantum thermodynamics

In this chapter, we discuss briefly the concepts of thermodynamics in quantum systems. We start with the definition of work in closed quantum systems. We then review the possibilies of how to calculate work and its fluctuations in open quantum systems. Last, we show how stochastic thermodynamics can be treated with the quantum jump method.

3.1 Definition of work in quantum systems

In classical systems, the system has always a well-defined energy. However, in quantum systems the energy is not always well-defined as the system state can be a superposition of energy eigenstates. For this reason, the classical treatment of stochastic thermodynamics cannot be straightforwardly extended into the quantum regime. These problems become particularly transparent when defining work. Classically, work can be defined in a closed system as the energy difference between the final state and the initial state:

$$W_{\mathrm{cl}}(x_\tau, x_0) = H(x_\tau, \tau) - H(x_0, 0), \tag{3.1}$$

where x_0 and x_τ are the initial and final system states in the phase space, H is the Hamiltonian function and the protocol starts at time 0 and ends at time τ. In the works of Bochkov and Kuzovlev in 1977 [14], Yukawa in 2000 [53] and Allahverdyan and Nieuwenhuizen in 2005 [54], the quantum version of Eq. (3.1) was introduced in the form of a work operator [31]:

$$\hat{W} = \hat{H}_H(\tau) - \hat{H}_H(0), \tag{3.2}$$

where the Hamiltonian functions are replaced with the Hamiltonian operators $\hat{H}$ and the subscript H denotes the Heisenberg picture. With the work operator, the moments of work are given by:

$$\langle \hat{W}^n \rangle = \mathrm{Tr}\{\hat{W}^n \hat{\rho}\}, \tag{3.3}$$

where $\hat{\rho}$ is the density matrix of the closed system. However, when calculating third and higher order moments of work, the work operator leads to problems due to the correlation functions that are not time-ordered [55]. These problems arise as the work operator approach treats work as a usual observable. However, as the work depends on both the final state and the initial state, it needs two energy measurements and thus it is not a usual quantum mechanical observable [29].

An alternative approach, called the two measurement protocol (TMP) was developed by Kurchan [33] and Tasaki [34] at the turn of the millenium. In TMP, the problem of possible energy superpositions is resolved by projective energy measurements at the beginning and at the end of the protocol. As a consequence, work is not defined as an operator but as a stochastic outcome of TMP:

$$W(E_f(\tau), E_i(0)) = E_f(\tau) - E_i(0), \tag{3.4}$$

where $E_i(0)$ is the energy outcome of the initial measurement and $E_f(\tau)$ is the energy outcome of the final measurement. For a closed system, the probability to measure state $|i(0)\rangle$ with energy $E_i(0)$ at time $t = 0$ and state $|f(\tau)\rangle$ with energy $E_f(\tau)$ at $t = \tau$ is given by [35]

$$P[f,i] = \mathrm{Tr}\{\hat{P}_{f(\tau)}\hat{U}(\tau,0)\hat{P}_{i(0)}\hat{\rho}_0\hat{P}_{i(0)}\hat{U}^\dagger(\tau,0)\hat{P}_{f(\tau)}\}, \tag{3.5}$$

where $\hat{U}(\tau,0) = \mathcal{T}_\leftarrow \exp\left(-\frac{i}{\hbar}\int_0^\tau dt\hat{H}(t)\right)$ is the unitary time evolution operator, $\mathcal{T}_\leftarrow$ describes the chronological time ordering and the projection operators are given by $\hat{P}_{i(t)} = |i(t)\rangle\langle i(t)|$, where $|i(t)\rangle$ is the state corresponding to the measurement result $E_i(t)$ at time t. The work generating function is obtained by Fourier transforming $P[f,i]$:

$$G(u) = \sum_{i,f} e^{iuW(E_f(\tau),E_i(0))}P[f,i] \tag{3.6}$$

$$= \mathrm{Tr}\{\mathcal{T}_\leftarrow e^{iu[\hat{H}_H(\tau)-\hat{H}_H(0)]}\bar{\hat{\rho}}_0\}, \tag{3.7}$$

where $\bar{\hat{\rho}}_0 = \sum_i \hat{P}_{i(0)}\hat{\rho}_0\hat{P}_{i(0)}$. The moments of work are then obtained by

differentiating $G(u)$ with respect to u at $u = 0$:

$$\langle W^n \rangle = (-i)^n \left. \frac{\partial^n G(u)}{\partial u^n} \right|_{u=0}. \tag{3.8}$$

When the initial density matrix is diagonal in the initial measurement basis, i.e., $\bar{\hat{\rho}}_0 = \hat{\rho}_0$, the time ordering $\mathcal{T}_{\leftarrow}$ in Eq. (3.7) is the only difference between the generating functions of TMP and work operator approaches. Due to time ordering, TMP avoids the non-time-ordered correlation functions that plague the work operator approach.

Let us assume that the system starts from thermal equilibrium such that the initial measurements yield a canonical density matrix

$$\bar{\hat{\rho}}_0 = \sum_i \frac{e^{-\beta E_i(0)}}{Z(0)} \left| i(0) \right\rangle \left\langle i(0) \right|, \tag{3.9}$$

where $Z(0) = \sum_i e^{-\beta E_i(0)}$ and $\beta = 1/(k_B T)$ is the inverse temperature. Taking into account that $\sum_i |i(t)\rangle\langle i(t)| = \hat{\mathbf{1}}$ and $\hat{U}(t,0)\hat{U}^\dagger(t,0) = \hat{\mathbf{1}}$ [30, 32], the average of $e^{-\beta W}$ can be expressed as

$$\langle e^{-\beta W} \rangle = e^{-\beta \Delta F}, \tag{3.10}$$

where $\Delta F = F(\tau) - F(0) = -(1/\beta) \log \left[Z(\tau)/Z(0) \right]$ is the Helmholtz free energy difference. This equation is known as the Jarzynski equality [15] and it assumes thermal equilibrium in the beginning of the protocol. For classical systems, the Jarzynski equality has been verified for closed and open systems. In the quantum regime, it has been experimentally verified only for closed quantum systems [36, 37]. In the experiment of Ref. [37], the work of a single realization is obtained using TMP. In Ref. [36], the TMP work generating function is measured with an ancilla system [56, 57].

Similarly to the classical case, the work done on a quantum system can also be calculated through the energy input into the system [30, 43, 58, 59]. For example, the first two TMP moments of work can be expressed as:

$$\langle W \rangle = \int_0^\tau \mathrm{Tr}\{[\partial_t \hat{H}(t)]_H \bar{\hat{\rho}}_0\} dt = \int_0^\tau \langle \hat{P}_H(t) \rangle, \tag{3.11}$$

$$\langle W^2 \rangle = 2 \int_0^\tau dt_1 \int_0^{t_1} dt_2 \mathrm{Re} \left\{ \langle \hat{P}_H(t_1) \hat{P}_H(t_2) \rangle \right\}, \tag{3.12}$$

where the power operator $\hat{P}(t) = \partial_t \hat{H}(t)$ describes *input power* injected into the system by the classical source. In some cases [29, 31, 35], the TMP

generating function of Eq. (3.7) has been casted into a form containing only the power operator due to a mistake in calculating the commutation relations [60]. For example in the celebrated article by Esposito et al. [35], the generating function is written as

$$G_0(u) = \mathbf{Tr}\left\{\mathcal{T}_{\rightarrow}\exp\left(i\frac{u}{2}\int_0^\tau dt\hat{P}_H(t)\right) \times \mathcal{T}_{\leftarrow}\exp\left(i\frac{u}{2}\int_0^\tau dt\hat{P}_H(t)\right)\bar{\hat{\rho}}_0\right\}, \tag{3.13}$$

which only gives correctly the first two moments of work. As shown in Publication I and in the consequent erratum [61] to the article [35], the correct form of Eq. (3.13) is given by

$$G(u) = \mathrm{Tr}\left\{\mathcal{T}_{\rightarrow}\exp\left(\int_0^\tau dt\sum_{n=1}^{\infty}(-1)^{n+1}\frac{(iu)^n}{n!2^n}\hat{B}_{n,H}(t)\right) \times \mathcal{T}_{\leftarrow}\exp\left(\int_0^\tau dt\sum_{n=1}^{\infty}\frac{(iu)^n}{n!2^n}\hat{B}_{n,H}(t)\right)\bar{\hat{\rho}}_0\right\}, \tag{3.14}$$

where the subscript H indicates the Heisenberg picture, $\hat{B}_1(t) = \hat{P}(t)$ and $\hat{B}_{n+1}(t) = \left[\hat{H}(t), \hat{B}_n(t)\right]$ for $n \geq 1$. We call the approach of calculating the work moments with Eq. (3.14) as the *power operator approach*[1]. As Eq. (3.14) is derived from Eq. (3.7) without additional assumptions, TMP and power operator approaches produce equivalent work moments for closed systems. Thus, the Jarzynski equality is also valid for the power operator approach.

Although the TMP definition of work has become the established treatment of work in quantum systems, it has its drawbacks. Most importantly, due to the initial energy measurement, the protocol always starts from an energy eigenstate. Consequently, it cannot describe work done in processes that start from an energy superposition. Such processes are common occurance in quantum information and computations [62–64]. To address these issues, several approaches have been recently proposed [64, 65].

[1]This approach differs from the power measurement scheme of Ref. [59], where the system evolution is altered by projecting the system into the eigenstates of the power operator at short intervals.

3.2 Work and fluctuation relations in open quantum systems

For a system coupled to a large environment, the projective measurements done in TMP become impractical due to the total system's large number of degrees of freedom. The projective measurements on the system degrees of freedom alone are not enough to obtain the work as also heat emitted into the environment must be taken into account. When the system-environment coupling is weak, this problem can be circumvented by continuously monitoring the heat emitted to the environment. This heat corresponds to the energy change in the environment and thus projective measurements on the entire environment are unnecessary.

If additionally the environment is infinite or memoryless, the system dynamics are usually modeled with the Lindblad equation. For the Lindblad equation, there are multiple approaches to calculate the work statistics. One of them is the generalized master equation, where a master equation similar to the Lindblad equation is derived for the work moments' generating function. Evolving this generalized master equation for multiple values of u in $G(u)$, the work distribution can be found. However, work in a single trajectory cannot be obtained.

In order to access the work done on a single realization, methods that unravel the Lindblad equation can be used, such as the quantum jump method [40]. In the next section, we show how the thermodynamics quantities and fluctuation relations can be calculated with the quantum jump method. These fluctuation relations can also be shown to hold for the Lindblad equation by using the stochastic Schrödinger equation [39] and the generalized master equation [35, 44, 45].

When the coupling between the system and the environment is strong, the energy of the total system cannot be obtained by measuring the energies of the system and the environment separately. Additionally, the dynamics cannot be described by the Lindblad equation. In this case, the work statistics can be obtained by treating the total system as a closed system. However, this is often computationally impossible due to the large size of the environment. Another approach is to model the environment as an infinite set of harmonics oscillators and use the Feynman-Vernon influence functional formalism [66]. The work moments or more generally entropy change can then be obtained by formulating a functional for

the entropy change [67] and the work moments' generating function (Eq. (3.7)) [68, 69] or by using the stochastic von Neumann-Liouville method [70] that unravels the Feynman-Vernon formalism as done in Refs. [2, 71].

3.3 Stochastic thermodynamics with quantum jump method

In order to access the work done on a single realization of the Lindblad equation [Eq. (2.10)], the quantum jump method offers a natural choice as it tries to mimic the trajectories realized in actual experiments. With this method, work can be calculated by associating each jump with heat exchange and by measuring the energy of the open quantum system at the beginning and at the end of the protocol.

For each trajectory, we denote the initial and final energy of the open quantum system as $E_i(0)$ and $E_f(\tau)$, respectively. Furthermore, let us use t_j to denote the time when the j:th jump occurs and $Q_j(t_j)$ to denote the heat emitted to the environment by the j:th jump. According to the first law of thermodynamics, the work is then given by

$$W = \Delta U + Q, \tag{3.15}$$

where $\Delta U = E_f(\tau) - E_i(0)$ is the internal energy change of the open quantum system, $Q = \sum_{j=1}^{N} Q_j(t_j)$ is the total heat emitted to the environment and N is the number of jumps in the trajectory. The probability of the trajectory is given by

$$\begin{aligned} &P_{QJ}[i, f, \{\hat{C}_{m_k}\}_{k=1}^{N}, \{t_k\}_{k=1}^{N}] \\ &= P_0[i] \left[\prod_{k=1}^{N} p^0(t_k, t_{k-1}) p_{m_k}(t_k) \right] p^0(\tau, t_N) P_\tau[f], \end{aligned} \tag{3.16}$$

where the protocol starts at time 0 and ends at time τ, $P_0[i]$ is the probability to start with the system state $|i\rangle$, $p_{m_k}(t_k)$ is the probability for a jump caused by the jump operator $\hat{C}_{m_k} = \sqrt{\Gamma_{m_k}} \hat{L}_{m_k}$ to occur during $[t_k, t_k + \delta t]$, $p^0(t_{k+1}, t_k)$ is the probability of no jump during the time-interval $[t_k, t_{k+1}]$ and $P_\tau[f]$ is the probability to measure the system state $|f\rangle$ at the end of the protocol. As shown in Publication II, we can use the protocol described in Section 2.4 to express Eq. (3.17) in a more elaborate form:

$$
\begin{aligned}
&P_{QJ}[i, f, \{\hat{C}_{m_k}\}_{k=1}^N, \{t_k\}_{k=1}^N] \\
&= (\delta t)^N P_0[i] \left[\prod_{k=1}^N \Gamma_{m_k}(t_k)\right] \times \\
&\left|\langle f|\hat{U}_{\text{eff}}(\tau, t_N)\left[\prod_{k=1}^N \hat{L}_{m_{N+1-k}}\hat{U}_{\text{eff}}(t_{N+1-k}, t_{N-k})\right]|i\rangle\right|^2,
\end{aligned}
\tag{3.17}
$$

where the no-jump evolution is given by

$$
\hat{U}_{\text{eff}}(t_{k+1}, t_k) = \mathcal{T}_{\leftarrow} e^{-\frac{i}{\hbar}\left[\int_{t_k}^{t_{k+1}} \hat{H}_{\text{eff}}(t) - i\frac{\hbar}{2}\sum_i \hat{C}_i{}^\dagger \hat{C}_i dt\right]} \tag{3.18}
$$

and $\hat{H}_{\text{eff}}(t)$ is the effective system Hamiltonian of the Lindblad equation. The probability distribution of work can then be obtained by associating each trajectory with a work value according to Eq. (3.15). If the jumps occur between the system eigenstates such that the jump operators have the form $\hat{L}_k(t) = \sum_{i,j} \alpha_{ij}(t) |i(t)\rangle \langle j(t)| \delta_{Q_k, E_j(t)-E_i(t)}$, then Q_k is the heat associated to the jump $\hat{L}_k$. We then obtain the probability distribution of work by taking the limit $\delta t \to 0$:

$$
\begin{aligned}
P(W) = &\sum_{i,f}\sum_{N=0}^{\infty}\sum_{\{\hat{C}_{m_k}\}_{k=1}^N} \frac{1}{N!}\prod_{i=1}^N \int_0^\tau dt_i \frac{1}{(\delta t)^N} \\
&\times P_{QJ}[i, f, \{\hat{C}_{m_k}\}_{k=1}^N, \{t_k\}_{k=1}^N]\delta[W - E_f(\tau) + E_i(0) - \sum_k Q_{m_k}(t_k)].
\end{aligned}
\tag{3.19}
$$

However, the Lindblad equation does not restrict the jump operators to act between the eigenstates of the system Hamiltonian. Thus, in general, it is possible to have jump operators between different superposition states without well defined energies. In these instances, it can be hard or even impossible to associate a work value with a given trajectory. We can still associate an entropy change to a trajectory. The only assumption needed is that the original Lindblad equation follows detailed balance between jump operators such that there exists a set of transition rates $\bar{\Gamma}_k$ such that

$$
\sum_k \Gamma_k(t)\hat{L}_k^\dagger(t)\hat{L}_k(t) = \sum_k \bar{\Gamma}_k(t)\hat{L}_k(t)\hat{L}_k^\dagger(t), \tag{3.20}
$$

where the summing is over all the jump operators. For example, this is satisfied if for each $\hat{C}_k = \sqrt{\Gamma_k}\hat{L}_k$ there exists another jump operator $\hat{C}_l = \sqrt{\Gamma_l}\hat{L}_l$ such that $\hat{L}_l = \hat{L}_k^\dagger$ [72].

The total entropy change of a trajectory can be defined as the ratio between the probabilities of the trajectory and its time-reversed trajectory. We can formulate the time-reversed counterpart for the forward trajectory of Eq. (3.17). In the time-reversed trajectory, we measure the system state $|f\rangle$ at the beginning ($\bar{t}=0$) and the system state $|i\rangle$ at the end ($\bar{t}=\tau$). In the time-reversed trajectory, all the jumps are reversed and they happen in reverse order, i.e., a jump caused by $\hat{C}_{\bar{m}_k}=(\bar{\Gamma}_{m_k})^{1/2}\hat{L}^\dagger_{m_k}$ occurs at a time $\bar{t}=\tau-t_k$, where the index $\bar{m}_k$ is related to the forward index m_k such that $\hat{L}_{\bar{m}_k}=\hat{L}^\dagger_{m_k}$. By demanding that the time-reversed no-jump evolution between jumps is given by $\hat{U}^\dagger_{\text{eff}}(t_{i+1},t_i)$, the probability for the reverse quantum jump trajectory can then be written as

$$\begin{aligned}&\bar{P}_{QJ}[f,i,\{\hat{C}_{\bar{m}_k}\}_{k=1}^N,\{\bar{t}_k\}_{k=1}^N]\\&=(\delta t)^N\bar{P}_0[f]\left[\prod_{k=1}^N\bar{\Gamma}_{m_k}(t_k)\right]\times\\&\left|\langle i|\left[\prod_{k=1}^N\hat{U}^\dagger_{\text{eff}}(t_k,t_{k-1})\hat{L}^\dagger_{m_k}\right]\hat{U}^\dagger_{\text{eff}}(\tau,t_N)|f\rangle\right|^2,\end{aligned}\tag{3.21}$$

where $\bar{P}_0[f]$ is the probability to start a reversed trajectory with the system state $|f\rangle$. The total entropy change is defined as the ratio of the forward and reversed trajectory probabilities:

$$\begin{aligned}&\Delta S_T[i,f,\{\hat{C}_{m_k}\}_{k=1}^N,\{t_k\}_{k=1}^N]\\&=\ln\left[\frac{P_{QJ}[i,f,\{\hat{C}_{m_k}\}_{k=1}^N,\{t_k\}_{k=1}^N]}{\bar{P}_{QJ}[f,i,\{\hat{C}_{\bar{m}_k}\}_{k=1}^N,\{\bar{t}_k\}_{k=1}^N]}\right]\\&=\ln\left\{\frac{P_0[i]}{\bar{P}_0[f]}\right\}+\ln\left[\prod_{k=1}^N\frac{\Gamma_{m_k}}{\Gamma_{\bar{m}_k}}\right].\end{aligned}\tag{3.22}$$

Due to the assumption that the jump operators follow detailed balance, the time-reversed trajectories correspond to the unraveling of the Lindblad equation

$$\begin{aligned}\frac{d\hat{\bar{\rho}}_S}{d\bar{t}}&=\frac{i}{\hbar}\left[\hat{H}_{\text{eff}}(\bar{t}),\hat{\bar{\rho}}_S(\bar{t})\right]\\&+\sum_{i=0}^M\left(\hat{\bar{C}}_i(\bar{t})\hat{\bar{\rho}}_S(\bar{t})\hat{\bar{C}}_i^\dagger(\bar{t})-\frac{1}{2}\left\{\hat{\bar{C}}_i^\dagger(\bar{t})\hat{\bar{C}}_i(\bar{t}),\hat{\bar{\rho}}_S(\bar{t})\right\}\right),\end{aligned}\tag{3.23}$$

where $\hat{\bar{C}}_i(\bar{t})=\sqrt{\bar{\Gamma}_i(\bar{t})}\hat{L}_i^\dagger(t)$. Equation (3.23) guarantees that the time-reversed trajectories are true quantum trajectories. Thus, the reversed trajectories' probabilities sum up to unity and it can be straightforwardly

shown that

$$\langle e^{-\Delta S_T} \rangle = 1, \tag{3.24}$$

where the average is over all the forward trajectories. Equation (3.24) is known as the integral fluctuation theorem of entropy change [16]. If the transition rates follow detailed balance such that $\Gamma_{m_k}/\bar{\Gamma}_{m_k} = e^{\beta Q_{m_k}}$ and the system starts from a canonical ensemble with temperature $T = 1/(k_B\beta)$, then the time-reversed trajectories can be chosen to start from a canonical ensemble with the same temperature. As a consequence, Eq. (3.24) simplifies to the Jarzynski equality:

$$\langle e^{-\beta W} \rangle = e^{-\beta \Delta F}, \tag{3.25}$$

where ΔF is the free-energy difference between the final and initial states and $\beta = 1/(k_B T)$.

4. Work fluctuations in weakly driven open quantum systems

In this chapter, we illustrate how to calculate the work statistics for an open quantum system that is weakly driven by a classical source. The results presented here are mainly based on Publication I with some results taken from Publication IV.

4.1 Master equation

We focus on a generic two-level system (qubit) with $\hat{H}_0 = \hbar\omega_0 \hat{a}^\dagger \hat{a}$ that is weakly driven by a classical source $\hat{V}_D(t) = \lambda(t)\hat{a}^\dagger + \lambda^*(t)\hat{a}$, where $\hat{a} = |0\rangle\langle 1|$ and $\hat{a}^\dagger = |1\rangle\langle 0|$ are the annihilation and creation operators in the undriven basis. The states $|1\rangle$ and $|0\rangle$ denote the excited and ground states of the undriven Hamiltonian, $\hat{H}_0$, respectively. Consequently, the system Hamiltonian is given by

$$\hat{H}_S(t) = \hat{H}_0 + \hat{V}_D(t). \tag{4.1}$$

The system is assumed to be coupled to an infinite bosonic environment by $\hat{V} = \sum_k \kappa_k(\hat{a}^\dagger \hat{b}_k + \hat{a}\hat{b}_k^\dagger)$, where the coupling strength κ_k is real and the operators $\hat{b}_k$ and $\hat{b}_k^\dagger$ are the bath annihilation and creation operators associated with energy ϵ_k, respectively. The environment Hamiltonian has the form $\hat{H}_E = \sum_k \epsilon_k \hat{b}_k^\dagger \hat{b}_k$. The total Hamiltonian is therefore given by

$$\hat{H}(t) = \hat{H}_S(t) + \hat{H}_E + \hat{V}. \tag{4.2}$$

Both the environment and interaction Hamiltonians are assumed to be time independent. This setup describes, for instance, a Cooper box coupled capacitively or a dc superconducting quantum interference device (dc-SQUID) coupled inductively to an infinite calorimeter [73].

As both the driving and the system-environment coupling are weak, we can treat them perturbatively. In a manner similar to Chapter 2, we can microscopically derive a Lindblad equation by invoking the Born-Markov and secular approximations[1]:

$$\begin{aligned}\frac{d\hat{\rho}_S}{dt} = &- \frac{i}{\hbar}\left[\hat{H}_S(t), \hat{\rho}_S(t)\right] \\ &+ \Gamma_\downarrow\left(\hat{a}\hat{\rho}_S(t)\hat{a}^\dagger - \frac{1}{2}\left\{\hat{\rho}_S(t), \hat{a}^\dagger\hat{a}\right\}\right) \\ &+ \Gamma_\uparrow\left(\hat{a}^\dagger\hat{\rho}_S(t)\hat{a} - \frac{1}{2}\left\{\hat{\rho}_S(t), \hat{a}\hat{a}^\dagger\right\}\right),\end{aligned} \tag{4.3}$$

where $\Gamma_\downarrow$ and $\Gamma_\uparrow = \Gamma_\downarrow e^{-\beta\hbar\omega_0}$ are the photon emission and absorption transition rates, respectively, and $\hat{\rho}_S(t)$ is the density matrix of the reduced system in the Schrödinger picture. In the Lindblad equation, we have neglected the third and higher order terms in $[\hat{V} + \hat{V}_D(t)]$. As a consequence, the jump operators act on the undriven states of the system.

4.2 Stochastic thermodynamics

As Eq. (4.3) is in the Lindblad form that satisfies Eq. (3.20), the integral fluctuation theorem of the entropy change $\langle e^{-\Delta S_T}\rangle = 1$ is satisfied with the total entropy change of a trajectory given by $\Delta S_T = \ln\left\{\frac{P_0[i]}{P_0[f]}\right\} + \ln\left[\prod_{k=1}^{N}\frac{\Gamma_{m_k}}{\Gamma_{\bar{m}_k}}\right]$ and the time-reverse trajectories correspond to the master equation:

$$\begin{aligned}\frac{d\hat{\bar{\rho}}_S}{d\bar{t}} = &+\frac{i}{\hbar}\left[\hat{H}_S(\bar{t}), \hat{\bar{\rho}}_S(\bar{t})\right] \\ &+ \Gamma_\downarrow\left(\hat{a}\hat{\bar{\rho}}_S(\bar{t})\hat{a}^\dagger - \frac{1}{2}\left\{\hat{\bar{\rho}}_S(\bar{t}), \hat{a}^\dagger\hat{a}\right\}\right) \\ &+ \Gamma_\uparrow\left(\hat{a}^\dagger\hat{\bar{\rho}}_S(\bar{t})\hat{a} - \frac{1}{2}\left\{\hat{\bar{\rho}}_S(\bar{t}), \hat{a}\hat{a}^\dagger\right\}\right),\end{aligned}$$

Consequently, the time-reversed transition rate of $\Gamma_\downarrow$ is $\Gamma_\uparrow$ and vice versa. As the transition rates follow detailed balance, the Jarzynski equality can be shown to hold when starting from thermal equilibrium:

$$\langle e^{-\beta W}\rangle = e^{-\beta\Delta F}, \tag{4.4}$$

where the work is defined such that the contribution from the driving has been neglected in the internal energy measurements and in the heat.

[1]For full derivation see Appendix B of Publication I.

That is, TMP measurements are done in the undriven basis and the heat emitted by a jump down (up) is assumed to be $\hbar\omega_0$ ($-\hbar\omega_0$). Equation (4.4) was shown to hold for a sinusoidal resonance driving in Ref. [40].

4.3 Comparison between TMP and power operator approach

In the previous section, the work was obtained using TMP measurements. However, work can be also calculated for open quantum systems with the power operator approach as described in Publication I. As the total system is closed, we can use the generating function of Eq. (3.14) to obtain the work moments. We only drive the system Hamiltonian and thus the derivative of the total Hamiltonian depends only on the system degrees of freedom. As a consequence, the first two work moments [Eq. (3.12)] can be calculated in the usual manner by using the master equation of the reduced density matrix as the operators in the correlation functions depend only on the system degrees of freedom [47, 55]. The higher moments however depend also on the environment degrees of freedom. For example, the third moment of work is given by

$$\begin{aligned}\langle W^3\rangle &= \langle W^3\rangle_0 + \frac{1}{4}\int_0^\tau dt \left\langle \left[\hat{H}_{S,H}(t), \left[\hat{H}_{S,H}(t), \hat{P}_H(t)\right]\right]\right\rangle \\ &\quad + \frac{3}{2}\int_0^\tau dt_1 \int_0^{t_1} dt_2 \mathbf{Re}\left\{\left\langle \hat{P}_H(t_1)\left[\hat{H}_{S,H}(t_2), \hat{P}_H(t_2)\right]\right\rangle\right\} \\ &\quad + \frac{1}{4}\int_0^\tau dt \left\langle \left[\hat{V}_H(t), \left[\hat{H}_{S,H}(t), \hat{P}_H(t)\right]\right]\right\rangle \\ \langle W^3\rangle_0 &= 3\int_0^\tau dt_1 \int_0^{t_1} dt_2 \int_0^{t_2} dt_3 \mathbf{Re}\left\{\left\langle \hat{P}_H(t_1)\hat{P}_H(t_2)\hat{P}_H(t_3)\right\rangle \right. \\ &\quad \left. + \left\langle \hat{P}_H(t_3)\hat{P}_H(t_1)\hat{P}_H(t_2)\right\rangle\right\}, \end{aligned} \tag{4.5}$$

where $\langle W^3\rangle$ is the third moment given by the general expression of Eq. (3.14) and $\langle W^3\rangle_0$ is the one given by Eq. (3.13). We can estimate the higher moments by invoking approximations similar to those used in the microscopic derivation of the master equation. In publication I, we study a two-level system that is sinusoidally driven with a frequency equivalent to that of the energy spacing, i.e., $\lambda(t) = \lambda_0 \sin(\omega_0 t)$. In Fig. 4.1, we compare the work moments obtained with the power operator approach to the ones generated by TMP. As seen from Fig. 4.1, TMP and power operator approach are in excellent agreement. Figure 4.1 also contains analytical approximations obtained by neglecting the fast oscillating terms of the

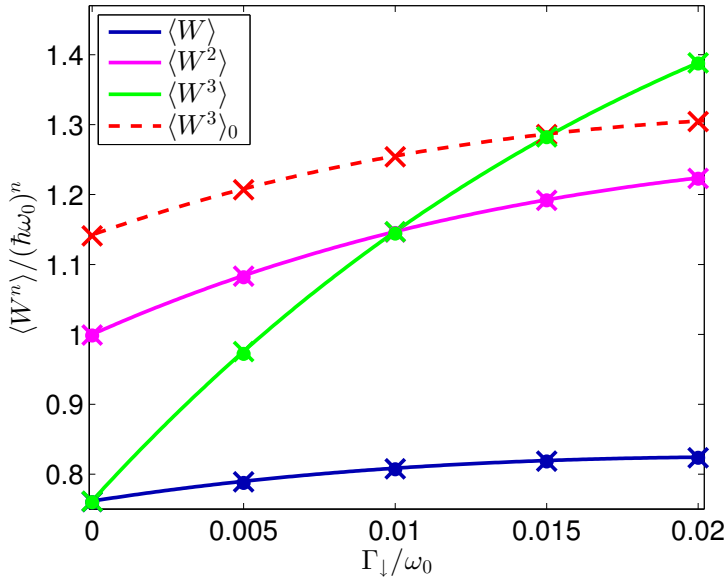

Figure 4.1. Comparison between the quantum jump method and master-equation results for the first three moments for different coupling amplitudes. The solid and dashed lines correspond to the analytical results where the fast oscillating terms of the drive are neglected, the dots correspond to the numerical quantum jump results, and the crosses correspond to the numerical master-equation data. The driving is assumed to be in resonance with ω_0, i.e., $\omega = \omega_0$, $\beta\hbar\omega_0 = 2.0$, $\lambda_0 = 0.05\hbar\omega_0$, and the drive lasts for 10 cycles, i.e., $\omega\tau = 20\pi$. The numerical results are calculated with 10^4 time steps. The quantum jump results consist of 10^6 realizations. The numerical master-equation and quantum jump results give a good agreement within the numerical accuracy: The largest difference in $\langle W^n \rangle / (\hbar\omega_0)^n$ is less than 0.0032.

drive and using the regression theorem [74]. The analytical results are accurate when the driving period τ consists of full or half cycles.

However, if the driving is slightly perturbed from the resonance, the TMP and power operator work values start to differ from each other. In Publication IV, we show that the difference between the average work of the two methods is given by

$$\begin{aligned} &\langle W_{\mathrm{TMP}} \rangle - \langle W_{\mathrm{P}} \rangle = \\ &-(\Gamma_\downarrow + \Gamma_\uparrow) \int_0^\tau dt \mathbf{Re}\{\lambda_I(t) \langle 0| \hat{\rho}_{S,I}(t) |1\rangle\}, \end{aligned} \tag{4.6}$$

where $\langle W_{\mathrm{TMP}} \rangle$ and $\langle W_{\mathrm{P}} \rangle$ denote the average work of TMP and power operator approach, respectively, $\hat{\rho}_{S,I}(t)$ is the system density matrix in the interaction picture with respect to $\hat{H}_0$. This difference is generally non-zero. For a resonant sinusoidal driving, the difference becomes zero if the fast

oscillating terms of the drive are neglected. This explains the excellent agreement in Fig. 4.1. For a slighly off-resonance driving $\lambda(t) = \lambda_0 \sin(\omega_d t)$ with $\omega_d = 1.0\omega_0 \pm 0.1\omega_0$, the difference between the work values becomes already significant, as discussed in Publication IV[2]. The difference is due to a different order of approximations in the derivation. In the calculation of TMP work values, the dynamics is assumed to strictly follow Eq. (4.3) and work is calculated assuming non-unitary evolution of the Lindblad equation. With the power operator approach, the dynamics is first assumed to be unitary at the beginning of the work calculations and only later the dynamics is approximated with the Lindblad equation. The difference between the work values highlights the importance of treating work consistently with the method that is used to describe the dynamics.

[2]In Publication IV, the simulations are done using a finite-size environment.

5. Work fluctuations in nearly adiabatically driven open quantum systems

In the previous chapter, we neglected the effect of driving on the dissipative part of the master equation and consequently on the work statistics. In this chapter, we take this into account by using the adiabatic renormalization prodecure.

5.1 Adiabatic renormalization

In Publication II, we use the adiabatic renormalization procedure [75, 76] to accurately take into account the effect of driving on the dissipation in the derivation of the master equation [77–79]. This allows us to take into account driving in the work statistics. The prodecure starts by diagonalizing the system Hamiltonian $\hat{H}_S$ in a time-independent basis $\{|m\rangle\}$. This is done by using an eigendecomposition such that the new diagonalized Hamiltonian reads as $\hat{\tilde{H}}_S^{(1)}(t) = \hat{D}_1^\dagger(t)\hat{H}_S(t)\hat{D}_1(t)$, where $\hat{D}_1(t)$ corresponds to the eigenproblem $\hat{H}_S(t)\,|m^{(1)}(t)\rangle = E_m^{(1)}(t)\,|m^{(1)}(t)\rangle$ with $\hat{D}_1\,|m\rangle = |m^{(1)}(t)\rangle$. The states $\{|m\rangle\}$ are usually referred to as diabatic. In a similar manner, we can transform the total density operator $\hat{\rho}(t)$ in the Schrödinger picture as $\hat{\tilde{\rho}}^{(1)}(t) = \hat{D}_1^\dagger(t)\hat{\rho}(t)\hat{D}_1(t)$. The evolution of $\hat{\tilde{\rho}}^{(1)}(t)$ is given by the effective Hamiltonian [78, 79]:

$$\hat{\tilde{H}}^{(1)}(t) = \hat{\tilde{H}}_S^{(1)}(t) + \hbar\hat{w}_1(t) + \hat{\tilde{V}}^{(1)}(t) + \hat{H}_E, \tag{5.1}$$

where $\hat{\tilde{V}}^{(1)}(t) = \hat{D}_1^\dagger(t)\hat{V}(t)\hat{D}_1(t)$ and $\hat{w}_1(t) = -i\hat{D}_1^\dagger(t)\partial_t\hat{D}_1(t)$.

Further transformations can be obtained by repeating the same procedure for the system part of the effective Hamiltonian [Eq. (5.1)], i.e, $\hat{\tilde{H}}_S^{(1)}(t)+\hbar\hat{w}_1(t)$. After n transformations, the corresponding density operator is written as $\hat{\tilde{\rho}}^{(n)} = (\hat{D}_S^{(n)})^\dagger\hat{\rho}\hat{D}_S^{(n)}$ with $\hat{D}_S^{(n)} = \prod_{i=1}^n \hat{D}_i = \hat{D}_1\hat{D}_2\cdots\hat{D}_{n-1}\hat{D}_n$.

The evolution of $\hat{\tilde{\rho}}^{(n)}$ is governed by an effective Hamiltonian

$$\hat{\tilde{H}}^{(n)} = \hat{\tilde{H}}_S^{(n)} + \hbar\hat{w}_n + \hat{\tilde{V}}^{(n)} + \hat{H}_E, \tag{5.2}$$

where $\hat{\tilde{H}}_S^{(n)} = \hat{D}_n^\dagger[\hat{\tilde{H}}_S^{(n-1)} + \hbar\hat{w}_{n-1}]\hat{D}_n$, $\hat{\tilde{V}}^{(n)} = (\hat{D}_S^{(n)})^\dagger \hat{V} \hat{D}_S^{(n)}$ and $\hat{w}_n = -i\hat{D}_n^\dagger \dot{\hat{D}}_n$. Each transformation forms a new set of time-dependent basis states $|m^{(n)}\rangle = \hat{D}_S^{(n)}|m\rangle$. For $n = 1$, these states correspond to the eigenstates of $\hat{H}_S$, referred to as the adiabatic states. For $n \geq 2$, the states correspond to the eigenstates of $\hat{D}_S^{(n-1)}[\hat{\tilde{H}}_S^{(n-1)} + \hbar\hat{w}_{n-1}](\hat{D}_S^{(n-1)})^\dagger$, referred to as the $(n-1)^{\text{th}}$-order superadiabatic states.

5.2 Master equation

In Publication II, we investigate a nearly adiabatically driven two-level system. We assume that the system is weakly coupled to the environment with the Hamiltonian $\hat{V}(t) = \hat{Y}(t) \otimes \hat{X}$, where $\hat{Y}(t)$ acts on the system degrees of freedom and $\hat{X}$ on the environment degrees of freedom. Let us denote the diabatic ground and excited states of the system as $|g\rangle$ and $|e\rangle$, respectively. As shown in Publication II, we can derive a master equation that depends on the number of basis transformations n by following the approach of Refs. [77–80]. By employing the Born-Markov and secular approximations, we obtain the following Lindblad equation for the system density matrix:

$$\begin{aligned}\dot{\hat{\rho}}_S = &-\frac{i}{\hbar}\left[\hat{H}_S, \hat{\rho}_S\right] \\ &+ \sum_{i=0}^{2}\left(\hat{L}_{(n,i)}\hat{\rho}_S\hat{L}_{(n,i)}^\dagger - \frac{1}{2}\left\{\hat{L}_{(n,i)}^\dagger\hat{L}_{(n,i)}, \hat{\rho}_S\right\}\right),\end{aligned} \tag{5.3}$$

where the error is of the third order in the coupling strength and linear order in the local (super)adiabatic parameter $\alpha_n = ||\hat{w}_n||/\omega_{01}^{(n)}$, where $||\hat{w}_n(t)|| = \sqrt{\mathrm{Tr}_S\{\hat{w}_n(t)^\dagger\hat{w}_n(t)\}}$, $\hbar\omega_{01}^{(n)} = E_e^{(n)} - E_g^{(n)}$ such that $E_e^{(n)} = \langle e|\hat{\tilde{H}}_S^{(n)}|e\rangle$ and $E_g^{(n)} = \langle g|\hat{\tilde{H}}_S^{(n)}|g\rangle$. In order for Eq. (5.3) to give an accurate approximation of the real dynamics, the local (super)adiabatic parameter must satisfy $\alpha_n \ll 1$. For nearly adiabatic driving, this condition is usually satisfied already with a rather low number of basis rotations. The jump

operators are given by

$$\begin{aligned}\hat{L}_{(n,0)} &= \sqrt{\Gamma_{(n,0)}}\,|g^{(n)}\rangle\,\langle e^{(n)}|\,,\\ \hat{L}_{(n,1)} &= \sqrt{\Gamma_{(n,1)}}\,|e^{(n)}\rangle\,\langle g^{(n)}|\,,\\ \hat{L}_{(n,2)} &= \sqrt{\Gamma_{(n,2)}}(|e^{(n)}\rangle\,\langle e^{(n)}| - |g^{(n)}\rangle\,\langle g^{(n)}|),\end{aligned} \tag{5.4}$$

where the transition rates are given by

$$\begin{aligned}\Gamma_{(n,0)} &= S(\omega_{01}^{(n)})|m_2^{(n)}|^2,\\ \Gamma_{(n,1)} &= S(-\omega_{01}^{(n)})|m_2^{(n)}|^2,\\ \Gamma_{(n,2)} &= S(0)|m_1^{(n)}|^2,\end{aligned} \tag{5.5}$$

where $m_1^{(n)} = \langle g^{(n)}|\hat{Y}|g^{(n)}\rangle = -\langle e^{(n)}|\hat{Y}|e^{(n)}\rangle$, $m_2^{(n)} = \langle g^{(n)}|\hat{Y}|e^{(n)}\rangle$, and $S(\omega)$ is the reduced spectral density of the noise source. In Publication II, we assume the noise spectrum to be ohmic such that $S(\omega) = 2\mu\omega/[\hbar(1 - e^{-\beta\hbar\omega})]$ [81], where μ is the damping constant related to the noise source. Furthermore, we introduce dephasing by assuming that $S(0) = 2\mu k_B T_0/\hbar^2$, where T_0 is the effective dephasing temperature.

5.3 Quantum thermodynamics for nearly adiabatically driven open quantum system

Similarly to Section 3.5, we can access to the distribution of work injected into the open quantum system during the driving protocol by utilizing the quantum jump method. For each trajectory, work is obtained as a combination of applying the two-measurement protocol to extract the internal energy of the system and allocating to each quantum jump event j the corresponding heat transferred to the environment $Q(t_j)$.

As discussed in Publication II, the number of basis rotations n directly affects the states between which the jumps occur. Each jump event corresponds to either an instantaneous collapse [see Eq. (5.4)] to the nth ground state [$\hat{L}_{(n,0)}$], an instantaneous collapse to the nth excited state [$\hat{L}_{(n,1)}$], or a phase flip [$\hat{L}_{(n,2)}$] within the nth (super)adiabatic basis. Similarly, we define the heat associated to a jump at $t = t_j$ to be $Q^{(n)}(t_j) = \hbar\omega_{01}^{(n)}(t_j)$ if the jump occurs along the $i = 0$ channel, by $Q^{(n)}(t_j) = -\hbar\omega_{01}^{(n)}(t_j)$ if it occurs along the $i = 1$ channel, and by $Q^{(n)}(t_j) = 0$ if it occurs along the $i = 2$ channel. Note that even though no heat transfer occurs along

the dephasing channel, it still contributes to the stochastic dynamics. The change in the trajectory-dependent internal energy is defined using TMP through projective measurements in the eigenbasis of $\hat{H}_S(t)$ such that $\Delta U = E_l^{(1)}(t_{\rm final}) - E_k^{(1)}(t_{\rm init})$, where k and l denote which eigenenergy was obtained at the initial and final time instances, respectively. The trajectory-dependent work corresponding to the $n^{\rm th}$-order dynamics is then given by

$$W^{(n)} = \Delta U + Q_{\rm tot}^{(n)}, \tag{5.6}$$

where the total heat is defined by $Q_{\rm tot}^{(n)} = \sum_j Q^{(n)}(t_j)$. The n-dependence of the stochastic dynamics is naturally inherited by the trajectory-dependent work through the heat exchange term. As the description of the dissipative dynamics becomes more accurate with increasing n, so does the heat allocated to each jump event. Consequently, the total heat $Q_{\rm tot}^{(n)}$ approaches the physically observable n-independent heat.

As Eq. (5.3) is of the Lindblad form with $\hat{L}_{(n,0)} \propto \hat{L}_{(n,1)}^\dagger$ and $\hat{L}_{(n,2)} = \hat{L}_{(n,2)}^\dagger$, the fluctuation theorem of entropy change can be shown to hold in a manner similar to that discussed in Section 2.4. As shown in Publication II, assuming that the system starts from thermal equilibrium, the integral fluctuation theorem simplifies to the Jarzynski equality for nearly adiabatic driving:

$$\langle e^{-\beta W^{(n)}} \rangle_{(n)} = e^{-\beta \Delta F}. \tag{5.7}$$

This equality always holds when the $n^{\rm th}$-order definition for the trajectory-dependent work is consistently used in association with the $n^{\rm th}$-order-order stochastic dynamics. In Publication II, we numerically verify this by studying a sinusoidally driven qubit with driving frequency $\omega_d = 0.3\omega_0$ and amplitude $\lambda = 0.5\hbar\omega_0$. Table 5.1 illustrates the results gotten with three driving cycles, i.e., $\Delta F = 0$. As seen from Table 5.1, the Jarzynski equality is valid only if the work definition is consistent with the dynamics.

	$n=2$	$n=1$	$n=0$
$\left\lvert 1-\langle e^{-\beta W^{(n)}}\rangle_{(n)}\right\rvert$	$(1\pm 3)\times 10^{-4}$	$(0\pm 4)\times 10^{-4}$	$(5\pm 7)\times 10^{-4}$
$\langle W^{(n)}\rangle_{(n)}/(\hbar\omega_0)$	$(693\pm 1)\times 10^{-4}$	$(969\pm 2)\times 10^{-4}$	$(3335\pm 1)\times 10^{-4}$
$\langle (W^{(n)})^2\rangle_{(n)}/(\hbar\omega_0)^2$	$(952\pm 2)\times 10^{-4}$	$(1373\pm 2)\times 10^{-4}$	$(5915\pm 3)\times 10^{-4}$
$\left\lvert 1-\langle e^{-\beta W^{(n)}}\rangle_{(2)}\right\rvert$	$(1\pm 9)\times 10^{-5}$	$(11\pm 9)\times 10^{-5}$	$(867\pm 6)\times 10^{-5}$
$\langle W^{(n)}\rangle_{(2)}/(\hbar\omega_0)$	$(6923\pm 3)\times 10^{-5}$	$(6901\pm 3)\times 10^{-5}$	$(5055\pm 3)\times 10^{-5}$
$\langle (W^{(n)})^2\rangle_{(2)}/(\hbar\omega_0)^2$	$(9507\pm 4)\times 10^{-5}$	$(9450\pm 4)\times 10^{-5}$	$(6473\pm 3)\times 10^{-5}$

Table 5.1. The exponentiated work and the first two moments of work using its n^{th}-order definition in conjunction with the dynamics of equal order (top rows) as well as that of $n=2$ (bottom rows). The top rows are calculated with 10^7 time steps, 2×10^7 trajectories for $n=1,2$ and 10^8 trajectories for $n=0$. The bottom rows are calculated with 10^6 time steps and 3×10^8 trajectories. The statistical uncertainty arising from averaging over the trajectories is estimated using the standard error of the mean, σ. In the table, the error estimates allow a maximum of 1.96σ deviation corresponding to a 95% confidence interval of the mean. Further details are presented in Publication II.

6. Finite environment quantum thermodynamics

In the previous chapters, we focused on scenarios where the dynamics can be modeled with the Lindblad equation. That is, we assumed an environment that is memoryless or infinite. In this chapter, we focus on quantum systems coupled to a large but finite environment. Consequently, the dynamics cannot be described by the Lindblad equation.

6.1 Motivation

To this day, only few experimentally realizable work measurement schemes have been proposed for open quantum systems [73, 82–84]. One of these is the calorimetric detection of the immediate environment [1, 73, 85]. In the calorimetric measurement scheme, heat exchange between the system and the environment is obtained by monitoring the environment's energy or effective temperature. However, in order to witness the changes in the environment's state, the environment has to be finite, i.e., in contrast to an ideal bath[1] it has to change its state when absorbing energy from the system. For this reason, the calorimetric setup cannot be modeled with the Lindblad equation as it neglects changes in the environment's state.

6.2 Model

Figure 6.1 presents a schematic illustration of the calorimetric setup. In the calorimetric measurement, a small quantum system is coupled to a

[1] We use *ideal bath* to denote an infinitely large or memoryless environment whose state is not affected by the system's evolution, i.e., the environment assumed in the derivation of the Lindblad equation.

large but finite environment. We assume the coupling between the system and the environment to be weak such that it can be neglected in the energy terms and modeled by stochastic jumps alone. Due to these environment induced jumps between the system eigenstates, heat is exchanged with the environment. The resulting changes in the environment energy are continuously monitored by a detector. As a consequence, the heat released to the environment can be measured without directly measuring the quantum system. As the environment is large and coupled to a detector, it is assumed to decohere quickly[2] into a set of energy eigenstates. We denote these eigenstates as microstate from here on.

In Publication IV, we derive a master equation for the calorimetric setup consisting of a two-level system (qubit) $\hat{H}_0 = \hbar\omega_0 \hat{a}^\dagger \hat{a}$ that is weakly driven by a classical source $\hat{V}_D(t) = \lambda(t)\hat{a}^\dagger + \lambda^*(t)\hat{a}$, where $\hat{a} = |0\rangle\langle 1|$ and $\hat{a}^\dagger = |1\rangle\langle 0|$ are the annihilation and creation operators in the undriven basis. The states $|1\rangle$ and $|0\rangle$ denote the excited and ground states of the undriven Hamiltonian, $\hat{H}_0$, respectively. The qubit Hamiltonian is then given by $\hat{H}_q(t) = \hat{H}_0 + \hat{V}_D(t)$. The qubit is coupled to a finite environment that we call as calorimeter from here on. We assume the calorimeter to consist of bosonic modes such that the calorimeter Hamiltonian is given by $\hat{H}_c = \sum_k \epsilon_k \hat{d}_k^\dagger \hat{d}_k$, where $\hat{d}_k$ and $\hat{d}_k^\dagger$ are the calorimeter's annihilation and creation operators associated with energy ϵ_k, respectively. The qubit and the calorimeter are assumed to be weakly coupled via the coupling Hamiltonian $\hat{V} = \sum_k \kappa_k(\hat{a}^\dagger \hat{d}_k + \hat{a}\hat{d}_k^\dagger)$.

6.3 Master equation

Due to the coupling to the detector and large but finite size of the calorimeter, we assume the calorimeter to decohere quickly into the einselected basis [87], such that the total density matrix of the qubit-calorimeter composite takes the form:

$$\hat{\rho}(t) = \sum_n \hat{\sigma}(n,t) \otimes |\Psi_n\rangle\langle\Psi_n| , \tag{6.1}$$

[2]That is, the decoherence is assumed to be faster than the other time scales such that the environment can be approximated with a decohered state between jumps. However, the decoherence is not assumed to occur infinitely fast as this would lead to the quantum Zeno effect [86].

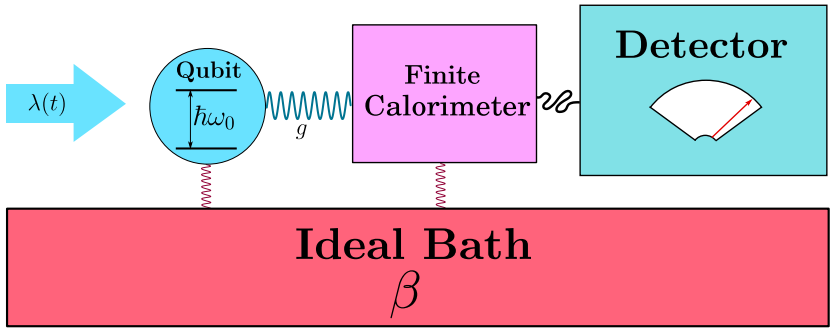

Figure 6.1. Schematic illustration of the calorimetric setup. The qubit and the calorimeter start from thermal equilibrium with an ideal bath. During the protocol, the qubit is driven by a classical field $\lambda(t)$. The calorimeter is constantly monitored with a detector.

where the qubit matrix $\hat{\sigma}(n,t)$ depends only on the qubit degrees of freedom. However, $\hat{\sigma}(n,t)$ cannot be interpreted as a qubit density matrix since its trace over qubit degrees of freedom does not give unity but the probability of a calorimeter state $|\Psi_n\rangle$. As shown in Publication IV, we can derive a master equation by invoking approximations similar to the ones done in the derivation of the Lindblad equation. However, the key difference is that instead of the Born approximation, we insert Eq. (6.1) in the integrand. This leads to the master equation:

$$\begin{aligned}\dot{\hat{\sigma}}(n,t) &= \frac{i}{\hbar}\left[\hat{\sigma}(n,t),\hat{H}_q(t)\right] \\ &- \sum_k \Bigg\{ \frac{\Gamma_{\uparrow,k}(n)}{2}\left[\hat{\sigma}(n,t)\hat{a}\hat{a}^\dagger + \hat{a}\hat{a}^\dagger\hat{\sigma}(n,t)\right] \\ &- \Gamma_{\downarrow,k}(n'_k)\hat{a}\hat{\sigma}(n'_k,t)\hat{a}^\dagger - \Gamma_{\uparrow,k}(n''_k)\hat{a}^\dagger\hat{\sigma}(n''_k,t)\hat{a} \\ &+ \frac{\Gamma_{\downarrow,k}(n)}{2}\left[\hat{\sigma}(n,t)\hat{a}^\dagger\hat{a} + \hat{a}^\dagger\hat{a}\hat{\sigma}(n,t)\right]\Bigg\}, \end{aligned} \tag{6.2}$$

where n'_k and n''_k are the calorimeter microstate indices that satisfy $|\Psi_{n'_k}\rangle = \hat{d}_k|\Psi_n\rangle / ||\hat{d}_k|\Psi_n\rangle||$ and $|\Psi_{n''_k}\rangle = \hat{d}_k^\dagger|\Psi_n\rangle / ||\hat{d}_k^\dagger|\Psi_n\rangle||$, respectively. Due to the terms with n'_k and n''_k, the evolution of $\hat{\sigma}(n,t)$ with different n are linked to each other. The transition rates depend on the state of the calorimeter and are of the form

$$\Gamma_{\uparrow,k}(n) = g_k^2 \langle\Psi_n|\hat{d}_k^\dagger\hat{d}_k|\Psi_n\rangle; \tag{6.3}$$

$$\Gamma_{\downarrow,k}(n) = g_k^2 \langle\Psi_n|\hat{d}_k\hat{d}_k^\dagger|\Psi_n\rangle, \tag{6.4}$$

with $g_k^2 = \frac{2\pi}{\hbar^2}\kappa_k^2\delta(\omega_0 - \epsilon_k/\hbar)$. From the point of view of the degrees of freedom of the qubit, Eq. (6.2) is non-Markovian as the evolution depends

both on the qubit's state and the state of the calorimeter.

We can also investigate the case when the calorimeter is not in a single microstate but a microcanonical ensemble. In this case, the decohered total density matrix reads

$$\hat{\rho}(t) = \sum_E \hat{\sigma}(E,t) \otimes \hat{\sigma}_c(E), \tag{6.5}$$

where E denotes the calorimeter energy and $\hat{\sigma}(E,t)$ is the qubit matrix. According to the microcanonical ensemble, the averaged calorimeter state $\hat{\sigma}_c(E) = [1/N(E)] \sum_k |\Psi_k\rangle \langle\Psi_k| \, \delta_{E_k,E}$, where E_k is the energy of microstate $|\Psi_k\rangle$ and $N(E)$ is the number of microstates with energy E. Let us call this averaged calorimeter state as a macrostate. The derivation of the corresponding master equation for $\hat{\sigma}(E,t)$ is similar to the previous case, yielding

$$\begin{aligned}
\dot{\hat{\sigma}}(E,t) &= \frac{i}{\hbar}\left[\hat{\sigma}(E,t), \hat{H}_q(t)\right] \\
&- \left\{ \frac{\Gamma_\uparrow(E)}{2}\left[\hat{\sigma}(E,t)\hat{a}\hat{a}^\dagger + \hat{a}\hat{a}^\dagger\hat{\sigma}(E,t)\right]\right. \\
&- \Gamma_\downarrow(E-\hbar\omega_0)\hat{a}\hat{\sigma}(E-\hbar\omega_0,t)\hat{a}^\dagger \\
&- \Gamma_\uparrow(E+\hbar\omega_0)\hat{a}^\dagger\hat{\sigma}(E+\hbar\omega_0,t)\hat{a} \\
&+ \left.\frac{\Gamma_\downarrow(E)}{2}\left[\hat{\sigma}(E,t)\hat{a}^\dagger\hat{a} + \hat{a}^\dagger\hat{a}\hat{\sigma}(E,t)\right]\right\},
\end{aligned} \tag{6.6}$$

where the transition rates are energy dependent

$$\Gamma_{\uparrow/\downarrow}(E) = [1/N(E)] \sum_{k,n} \Gamma_{\uparrow/\downarrow,k}(n)\delta_{E_n,E}. \tag{6.7}$$

6.4 Finite environment quantum jump model

In Publication III, we derive a quantum jump model equivalent to the master equation of Eq. (6.2). Let us denote this model as the finite-environment quantum jump (FEQJ) model to distinguish it from the standard quantum jump method. In FEQJ model, the interaction between the qubit and the calorimeter is described by stochastic jumps. When a jump occurs, both the qubit and the calorimeter states change such that the energy difference of the calorimeter states corresponds to the energy change in the qubit. For the system studied, these jumps are caused by jump operators $\hat{D}_{\downarrow,k} = g_k\hat{a} \otimes \hat{d}_k^\dagger$ and $\hat{D}_{\uparrow,k} = g_k\hat{a}^\dagger \otimes \hat{d}_k$. For convenience, we denote the jump operators using only one index $\hat{D}_m$.

Let us assume that the calorimeter is in a microstate $|\Psi_n\rangle$ and the qubit is in a state $|\psi(t)\rangle$ at time t. We define the probability for a transition in the time interval $[t, t+\delta t]$ as

$$\delta p = \sum_m \delta p_m = \sum_m \delta t \mathbf{Tr}_{q+c}\{\hat{D}_m^\dagger \hat{D}_m \hat{\sigma}_q \otimes \hat{\sigma}_c\}, \tag{6.8}$$

where δp_m is the probability for a jump corresponding to the jump operator $\hat{D}_m$, $\hat{\sigma}_q(t) = |\psi(t)\rangle\langle\psi(t)|$ is the matrix form of the qubit state, and $\hat{\sigma}_c(t) = |\Psi_n(t)\rangle\langle\Psi_n(t)|$ is the instantaneous calorimeter microstate, and the trace is over both the qubit (q) and calorimeter (c) degrees of freedom. If a jump corresponding to $\hat{D}_m$ occurs, the new qubit and calorimeter states are given by $\hat{\sigma}_q(t+\delta t) = \mathrm{Tr}_c\{\hat{D}_m\hat{\sigma}_q\otimes\hat{\sigma}_c\hat{D}_m^\dagger\}/(\delta p_m/\delta t)$ and $\hat{\sigma}_c(t+\delta t) = \mathrm{Tr}_s\{\hat{D}_m\hat{\sigma}_q\otimes\hat{\sigma}_c\hat{D}_m^\dagger\}/(\delta p_m/\delta t)$.

If no jumps occur during the time interval $[t, t+\delta t]$, the time evolution is governed by the non-unitary Hamiltonian

$$\hat{H}(t) = \hat{H}_q(t) + \hat{H}_c - \frac{i\hbar}{2}\sum_m \hat{D}_m^\dagger \hat{D}_m, \tag{6.9}$$

where $\hat{H}_q$ and $\hat{H}_c$ are the qubit and calorimeter Hamiltonians, respectively. The new qubit state $\hat{\sigma}_q(t+\delta t) = \mathrm{Tr}_c\{\hat{U}(t+\delta t,t)\hat{\sigma}_q\otimes\hat{\sigma}_c\hat{U}^\dagger(t+\delta t,t)\}/(1-\delta p) + \mathcal{O}(\delta t^2)$, where $\hat{U}(t+\delta t,t) = 1 - \frac{i}{\hbar}\hat{H}(t)\delta t$. Similarly, the new calorimeter state $\hat{\sigma}_c(t+\delta t) = \mathrm{Tr}_s\{\hat{U}(t+\delta t,t)\hat{\sigma}_q\otimes\hat{\sigma}_c\hat{U}^\dagger(t+\delta t,t)\}/(1-\delta p) + \mathcal{O}(\delta t^2)$, which gives $\hat{\sigma}_c(t+\delta t) = \hat{\sigma}_c(t)$ as we assumed that $\hat{\sigma}_c(t)$ is in a microstate. As a consequence, it is sufficient to focus in detail only on the system dynamics, where the calorimeter's state only affects the transition rates. That is, we can use the calorimeter traced jump operators defined as $\hat{C}_{\uparrow,m}(n) = \sqrt{\Gamma_{\uparrow,m}(n)}\hat{a}^\dagger$ and $\hat{C}_{\downarrow,m}(n) = \sqrt{\Gamma_{\downarrow,m}(n)}\hat{a}$. As proven in Publication IV, an average over all the trajectories produces a density matrix evolution equivalent to Eq. (6.2).

In many systems such as in electronic devices [88, 89], the relaxation rate inside the calorimeter is the fastest time scale. Consequently, the calorimeter relaxes into a macrostate immediately after jump. FEQJ model can be used by summing over all the transition rates corresponding to the same energy change. This leads to calorimeter traced jump operators of the form $\hat{C}_\uparrow(E) = \sqrt{\Gamma_\uparrow(E)}\hat{a}^\dagger$ and $\hat{C}_\downarrow(E) = \sqrt{\Gamma_\downarrow(E)}\hat{a}$, where E is the energy of the calorimeter. The master equation (6.6) is recovered by averaging over all the trajectories, as shown in Publication IV.

6.5 Fluctuation theorems

The total system is initially prepared such that both the qubit and the calorimeter start as a pure state given by the joint probability $P[i, \Psi_0]$, where $|i\rangle$ and $|\Psi_0\rangle$ are the initial qubit and calorimeter states, respectively. Due to the energy change with the qubit, the calorimeter can jump to a different microstate such that the energy difference between the microstates corresponds to the energy change in the qubit. For each trajectory, we can define a corresponding reverse trajectory as done in Publication III in a fashion similar to Section 3.3. The reversed trajectory starts with the final qubit and calorimeter states of the forward trajectory and has reversed jumps. As commonly done in stochastic thermodynamics [90, 91], we can define the entropy change associated with a jump as the logarithmic ratio of the forward and backward transition rates. Due to the symmetry $\Gamma_{\downarrow,m}(\Psi_k) = \Gamma_{\uparrow,m}(\Psi_{k+1})$, this entropy change is always zero if the calorimeter stays in a single microstate between the jumps. Thus, the total entropy change of a trajectory depends only on the initial and final states of the qubit and the calorimeter, i.e.,

$$\Delta S_T = \ln \left\{ P[i, \Psi_0] / \bar{P}[f, \Psi_N] \right\}, \tag{6.10}$$

where $\bar{P}[f, \Psi_N]$ is the probability to start a reversed trajectory with the final qubit state $|f\rangle$ and the final calorimeter state $|\Psi_N\rangle$ of the forward trajectory. The total entropy change then satisfies the fluctuation theorem:

$$\langle e^{-\Delta S_T} \rangle = 1, \tag{6.11}$$

where the average is over all the forward trajectories. If the initial probability distribution of the forward trajectory follows the canonical ensemble in equilibrium with an ideal heat bath, the probability distribution of the reversed trajectories can be chosen to follow a canonical ensemble with the same temperature. By defining the work W associated with a single trajectory as the energy difference between the final and initial states of the qubit-calorimeter composite, Eq. (6.11) gives the Jarzynski equality for work as

$$\langle e^{-\beta W} \rangle = e^{-\beta \Delta F}, \tag{6.12}$$

where ΔF is the free-energy difference between the final and initial states.

From the stochastic thermodynamics point of view, the situation where the calorimeter relaxes into a microcanonical ensemble is more interesting. In this case, the transition rates satisfy a detailed balance condition

$$\Gamma_{\downarrow}(E-\hbar\omega_0)/\Gamma_{\uparrow}(E) = N(E)/N(E-\hbar\omega_0), \tag{6.13}$$

which resembles the fluctuation relation derived for microcanonical ensembles [92–97]. The entropy change of a jump up with the calorimeter energy E is given by

$$\Delta s_{\uparrow}(E) = -\ln\left(\frac{\Gamma_{\downarrow}(E-\hbar\omega_0)}{\Gamma_{\uparrow}(E)}\right) = \ln\left(\frac{N(E-\hbar\omega_0)}{N(E)}\right), \tag{6.14}$$

which has a natural interpretation as the Boltzmann entropy change of the calorimeter. The entropy change of up and down jumps are related by $\Delta s_{\uparrow}(E) = -\Delta s_{\downarrow}(E-\hbar\omega_0)$. The probability to start with the qubit state $|i\rangle$ and the calorimeter macrostate of energy E_0 is given by $P[i, E_0]$. The total entropy change is then given by

$$\Delta S_T = \ln\left\{P[i,E_0]/\bar{P}[f,E_N]\right\} + \sum_{i=1}^{N}\Delta s_{\chi_i}(E_{i-1}), \tag{6.15}$$

where N is the number of jumps, E_i is the calorimeter energy after the i^{th} jump, $\chi_i = \uparrow / \downarrow$ is the direction of i^{th} jump, and $\bar{P}[f, E_N]$ is the probability to start a reversed trajectory with the forward trajectory's final qubit state $|f\rangle$ and calorimeter energy E_N. As Eq. (6.11) still holds, we recover the Jarzynski equality if we start from the canonical ensemble. Figure 6.2 presents numerical results with a sinusoidally driven qubit coupled to harmonic oscillators with an energy gap equivalent to that of the undriven qubit. In the simulations, the calorimeter is assumed to relax into a microcanonical ensemble immediately after a jump. As can be seen from Fig. 6.2(d), the Jarzynski equality is valid independent of the number of harmonic oscillators although the work distribution depends on the number of them. In Ref. [3], we investigated a setup where the heat emission to the ideal bath is allowed during the drive. For the setup, the Jarzynski equality is again valid when the necessary conditions are satisfied.

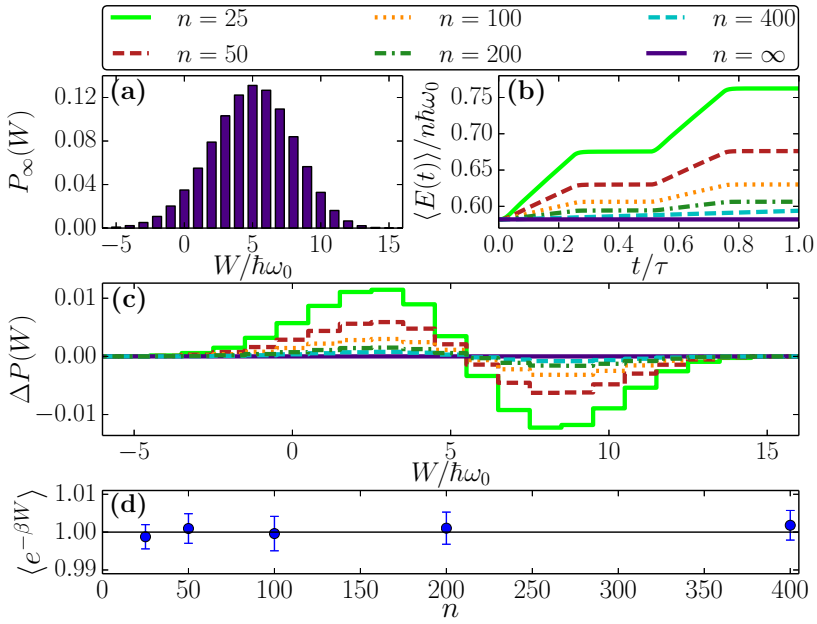

Figure 6.2. Influence of finite-size calorimeter on the work and energy statistics when it consists of n harmonic oscillators. (a) The probability distribution of work in the case of $n = \infty$, $P_\infty(W)$. (b) Time evolution of the average calorimeter energy for different values of n. (c) Deviation of the probability distribution of work $\Delta P(W) \equiv P_n(W) - P_\infty(W)$. (d) Numerical verification of the Jarzynski equality. The error bars are the standard deviation times 1.96 and correspond to a 95 % confidence interval. Further details are presented in Publication III.

7. Summary and conclusions

This thesis has focused on work statistics and fluctuation relations in open quantum systems. In all the results presented in the thesis and Publications I-IV, we have assumed the coupling to be weak between the system and the environment. In Chapters 2 and 3, we gave a short introduction to the dynamics of open quantum systems and quantum thermodynamics, respectively.

Chapter 4 summarized the findings of Publication I. We showed that the TMP and power operator work definitions agree in the case of a weakly and sinusoidally driven two-level system if the driving frequency is in resonance with the energy gap of the system. However, there exists a difference between the definitions in the case of off-resonance driving. This is due to a different order of approximations when advancing from the total system's unitary evolution to the non-unitary evolution caused by the Lindblad equation. In the case of a closed system, both definitions agree.

In Chapter 5, we used the adiabatic renormalization procedure to study work statistics in the case of a strongly but slowly driven two-level system. Based on Publication II, we showed that the Jarzynski equality holds only if the work is defined consistently with the number of basis transformations used in the dynamics. This is important from the point of view of the experiments, where often only the jump time distribution [98–101] is obtained instead of the heat transfer associated to each jump. In this case, the evaluation of the work distribution must externally impose to each detected jump event the corresponding heat transfer and, accordingly, adopt a definition for the trajectory-dependent work. Depending on the adopted definition, the Jarzynski equality may or may not be accurately retrieved using the experimental jump time distribution.

In Chapter 6, we focused on the influence of finite environment on the dynamics and thermodynamics of open quantum systems. The finite environment plays an important role in the experimental measurement of work in open quantum systems. In open quantum systems, the measurement of the internal energy of the system is not enough, also the heat released to the environment must be detected. In order to monitor the heat exchange, the emission or absorption of heat must leave traces on the state of the environment. That is, the changes in the environment's state must be large enough to be experimentally detected. In the case of an infinitely large environment, these changes become non-existent and therefore impossible to detect. However, if the environment is finite, the changes in the environment's state also affect the system's evolution. For this reason, the usual Lindblad equation and it's stochastic unravelings are unsuited to describe the dynamics accurately.

In Chapter 6, we summarized the findings of Publications III-IV. We showed that a master equation resembling the Lindblad equation can be derived for the setup by assuming that the environment decoheres quickly into its eigenstates. Additionally, we developed a finite quantum jump method that unravels the master equation into stochastic trajectories that depend on their own history through the state of the environment. Therefore, from the point of view of the system degrees of freedom, the trajectories are non-Markovian. We showed that the common fluctuation relations are valid when their necessary conditions are satisfied. We studied both the cases, where the environment stays in a single eigenstate or a microcanonical ensemble between jumps. If the environment is assumed to be in a microcanonical ensemble, we showed that the entropy change caused by a jump can be linked to the change in the environment's Boltzmann entropy similarly to the studies of fluctuation relations in closed microcanonical ensembles [92–97].

In this thesis, we have focused mostly on the work statistics. However, a lot of research has been done on information thermodynamics in classical and quantum systems [102–105]. One future research direction is to use the finite-environment model developed in this thesis to study feedback and measurement operations together with environment engineering. The formalism presented here offers a theoretical framework to study much more complicated feedback routines than usually done with

information thermodynamics [105, 106]. It also includes implicitly the measurement caused by the environment rendering the additional measurement operations unnecessary.

Another research direction is to study how the trajectory based definition of non-Markovianity used in this thesis connects to the measures of non-Markovianity like the BLP-measure [107] used in quantum information [108].

Lately, the quantum heat engines and other thermodynamic machines have been studied extensively [10, 109–117]. Already the first experimental realization of such device has been made [10]. The analysis of these devices commonly focuses on the use of averages to describe the performance. The finite-environment formalism presented in this thesis could be used to optimize the environment and feedback to gain higher efficiency. The efficiency of a device is usually calculated as the ratio of the averaged output work and the averaged input work. However, as discussed in this thesis, the average is not enough to describe the performance as the shape of the distribution also matters. Even if two devices might have the same efficiency, a measure should be created to distinguish the smoothly functioning quantum engine from the one working sporadically.

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Aalto-DD 15/2017

ISBN 978-952-60-7264-7 (printed)
ISBN 978-952-60-7263-0 (pdf)
ISSN-L 1799-4934
ISSN 1799-4934 (printed)
ISSN 1799-4942 (pdf)

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