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„Charging Precision For Finite-Dimensional Quantum Batteries “

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Abstract

Quantum thermodynamics is a field which attempts to understand the connection between the laws of thermodynamics, which largely govern macroscopic processes and the microscopic description provided by quantum mechanics. One topic of importance in this field, which is of central interest for this thesis, is the task of energy extraction from and energy charging into small, thermally isolated, quantum mechanical systems, we call *quantum batteries*.
Since both, extraction and charging processes considered in this thesis are performed by unitary operations, there is no heat flow resulting in the fact that that work alone is responsible for any change of the energy in these batteries. This gives rise to a new set of questions such as 'What exactly constitutes work on the quantum scale?' or 'What are fundamental thermodynamic bounds valid on the micro- or nonoscale?'.
Finally, the central goal of this thesis is to develop a unitary battery charging protocol based on the works of N. Friis and M. Huber in [1]. While the protocol proposed in [1] considers a more general case of infinite-dimensional systems, the protocol proposed in this thesis allows us to study the dynamics of charging a finite-dimensional quantum battery. The purpose of the proposed protocol is to use sequences of (non-unique) unitary, two-level rotations that raise the average energy of a finite-dimensional quantum battery initially in a completely passive state, while additionally minimizing the energy variance of the final state.
Our analysis shows, that the proposed protocol, can lead to an increase or decrease in variance in the battery depending on the input energy and temperature. But generally speaking, for non-zero initial temperatures, a trend of decreasing variance can be observed if the battery has been charged to half of its maximal capacity or less. Charging the battery any further than that, results in a trend of increasing variance.

Zusammenfassung

Das Feld der Quantenthermodynamik versucht die Verbindung zwischen den Gesetzen der Thermodynamik, welche großteils makroskopische Prozesse beschreiben und den Vorhersagen der Quantenmechanik, einer Theorie die sich mit Teilchen auf kleinsten Skalen befasst, zu verstehen. Ein wichtiges Thema in diesem Bereich ist das Extrahieren (von Energie) und Aufladen (durch Energie) von kleinen, thermisch isolierten, quanten mechanischen Systemen, die wir als *Quantenbatterien* bezeichnen.
Weil die Extraktions- und Aufladungsprozesse in dieser Arbeit ausschließlich durch unitäre Operationen durchgeführt werden, gibt es keinen Wärmefluss, was bedeutet, dass Arbeit allein für die Änderung der Energie der Batterie verantwortlich ist. Diese Aufgabestellung führt zu einem neuen Set von Fragen wie 'Was genau macht Arbeit in der Quantenmechanik aus?' oder 'Was sind fundamentale thermodynamische Limits auf der Mikro- oder Nanoskala?'
Der Schwerpunkt dieser Masterarbeit ist die Entwicklung eines Protokolls, welches auf der Arbeit von N. Friis und M. Huber in [1] basiert und durch unitäre Operationen eine Quantenbatterie aufladen kann. Während das vorgeschlagene Protokoll in [1] den allgemeineren Fall eines unendlich-dimensionalen Systems betrachtet, erlaubt uns das Protokoll welches in dieser Arbeit vorgestellt wird, die Dynamik des Aufladevorgangs für endlich-dimensionale Quantenbatterien zu untersuchen. Das Ziel des Protokolls ist es durch Sequenzen von (nicht eindeutigen) unitären Rotationen die Energie einer endlich-dimensionalen Quantenbatterie, welche ursprünglich in einem *komplett passiven* Zustand war, zu erhöhen, während man zusätzlich die Varianz der Energie des Endzustandes minimiert.
Unsere Untersuchung zeigt, dass das unser Protokoll, zu einer Verringerung oder Steigerung der Varianz in der Batterie führen kann, abhängig von der Energie mit der geladen wird und der Temperatur. Allerdings kann generell gesagt werden, dass für endliche Temperaturen die Varrianz eine fallende Tendenz hat, wenn die Batterie bis zur Hälfte ihrer maximalen Kapazität geladen wird. Ladet man eine Batterie weiter als bis zur Hälfte auf, wird die Varianz tendenziell steigen.

Chapter 1

Introduction

1.1 Quantum Thermodynamics

The rise of quantum mechanics in the 20^{th} century induced a revolution across many fields of science, which led among others to inventions such as semiconducting transistors or lasers [2]. Considering the speed of the resulting miniaturization of technology one could say in retrospect that it was just a matter of time until scientists would start to investigate thermal machines and engines on the quantum scale [3][4][5]. This premise led to the study of the applicability of the laws of thermodynamics on the quantum scale [6][7][8], which gave rise to a field called *quantum thermodynamics*. Broadly speaking quantum thermodynamics is a field which attempts to understand the connection between the microscopic description provided by quantum mechanics and the macroscopic laws of thermodynamics [9][10].

An excellent example for this is provided by the process of thermalization, which all of us know from our daily lives. Leave a hot cup of coffee in a closed room and immediately it will start cooling down until it has reached room temperature [11]. This fundamental fact of nature becomes less and less clear as we move into the quantum regime. Quantum thermodynamics attempts to describe how this process, emerges from quantum mechanical dynamics [10]. Ideally we would expect this behavior to emerge from our most basic laws such as Newton's or Schrödinger's equations. However, the process of thermalization itself can and must be broken down in the quantum regime into multiple, different aspects which have to be studied separately. N. Linden et al. were able to show in [12] that equilibration itself to some degree is a universal property of large quantum systems.

Additionally we will now list some of the other important topics which concern quantum thermodynamics:

- **Resource Theories**

  Resource Theories are generally concerned with managing a valuable resource as efficiently as possible. For this task one needs to define a resource, a class of *free operations* that can be implemented at no cost and *free states*, which can be generated at no cost. With these at hand one can study what kind of state transformations for the free initial states are possible by making use of the free operations. Additionally, the same free operations can realize more state transformations by having access to the valuable resource than without [13][6].

  Considering thermal interactions as a resource, energy preserving unitary operations as free operations and Gibbs states as free states allows us to study thermodynamical quantities in the quantum regime.

- **Quantum fluctuation relations**

  Statistical physics was able to show that the macroscopic parameters of thermodynamics can be interpreted as averages of microscopic processes. As with any average it comes with a probability distribution and its corresponding fluctuations of the specific values. Generally, these fluctuations are so small on the macroscopic scale that they are effectively negligible. However, the situation changes drastically in the quantum regime. How can thermodynamics be properly described in a domain where quantum fluctuations cannot be ignored [14][9][8]?

- **Quantum thermal machines and engines**

  As stated before it was the desire to consider thermal machines and engines in the quantum regime which gave rise to the field of quantum thermodynamics that as we have seen eventually grew into much more. This, now sub-field, deals with the optimization of various tasks performed on quantum versions of engines such as batteries which shall be the focus of this thesis [4][15][16][17] [1][18].

1.2 Motivation

Batteries play an indispensable role in our daily lives. However, the miniaturization of technology requires us to consider batteries on increasingly small scales, where eventually thermal and quantum fluctuations become non-negligible, eventually giving rise to the concept of *quantum batteries* (QBs), introduced by R. Alicki and M. Fannes in [19]. In this thesis we will define QBs as thermally isolated, quantum mechanical systems from which work can be extracted or into which work can be charged using specific processes. Thus, a major part of this thesis will be devoted to the study of different extraction and charging protocols.

Additionally, we will analyze the fact that in the quantum regime fluctuations stemming from quantum and thermal effects make a clear definition of thermodynamic quantities such as work hard [9]. We will discuss different approaches proposed in [9], [20] and [21], which attempt to estimate these fluctuations and compare them to each other.

Finally, the central goal of this thesis is to develop a unitary battery charging protocol, which is an extension of the work by N. Friis and M. Huber in [1]. The goal of the protocol is to raise the average energy of a finite-dimensional quantum battery, while additionally minimizing the energy variance of the final state. To this end we will consider specific sequences of unitary, two-level rotations ensuring that the final state is in the unitary orbit of the initial state. Our results will show that the proposed protocol can lead to a decrease of variance when compared to the initial state for non-zero temperatures. Generally speaking a trend of decreasing variances can be observed for any input energy up until the battery has been charged to half of its maximal capacity. In contrast to the infinite-dimensional case in [1], where the battery has no maximal capacity, charging the battery past this amount will result in a trend of increasing variances. This result then remains valid for all finite dimensions.

Additionally, we will calculate a 'boundary' temperature that denotes a temperature for which the curve for the minimal variance in 4.7 (a) is always below the initial variance. This behavior is then also true for any temperature above the 'boundary' temperature for the same dimension.

1.3 Structure

This thesis is structured into three main chapters: In chapter 2 we will establish the tools necessary for understanding the extraction and charging protocols, which will be considered in chapter 4. Concepts such as passivity and complete passivity will arise when we consider a work extraction process for thermally isolated systems in 2.3 and 2.4.

In chapter 3 we will review the problems associated with characterizing work in the quantum regime and discuss the advantages and disadvantages of three different approaches. The operator of work 3.3, the TPM scheme 3.4 and quasi-probabilities 3.6 will be investigated and we will see that each approach fails to satisfy all desired conditions for complete work characterization. Additionally, we will discuss in 3.5 a no-go result proposed by M. Perarnau-Llobet et al. in [22], which argues that our inability to completely characterize work does not come from our lack of knowledge but is of fundamental nature.

Finally chapter 4 can be divided into two parts. In the first part 4.1-4.4.2 we will discuss the specifics of different extraction and charging protocols. In the second part 4.5 we will present a detailed description of a unitary battery charging protocol for finite-dimensional systems with equally spaced energy levels. While [1] deals with the more general case of infinite-dimensional quantum batteries, the extension proposed in this thesis allows us to study the dynamics of charging finite-dimensional quantum batteries.

Chapter 2

Establishing Foundations

In this chapter we will formulate some basic relations that are important for this thesis such as the first and second law of thermodynamics and define central quantities like heat Q or Work W. Later we will apply this knowledge to investigate the basics of work extraction in the quantum regime discussed in [16][17]. We will do so while relying on the rather standard textbook notation of [23][24][11].

Additionally, concepts like passivity, complete passivity and entanglement will be introduced in sections 2.4 and 2.5. The goal of this chapter is to provide the reader with helpful tools which will be useful for understanding the following chapters in this thesis.

2.1 First Law of Thermodynamics

Before we begin let us go through an example of a quantum particle trapped in a double well potential [25]. This means that it can move freely from one end to the other but is surrounded by infinitely high potential walls as displayed in Fig.2.1. In quantum mechanics a *state*, represented in the simplest case by a d-dimensional vector $|\psi\rangle$, contains all accessible information in a quantum mechanical system. The state vector $|\psi\rangle$ is a normalized vector in the Hilbert space, which means that $|\psi\rangle \in \mathcal{H}^d$, where $\mathcal{H}^d$ is an abstract vector space that

- is a linear vector space, with scalar product in $\mathbb{C}$, which means that its elements are vectors with complex components which can be added to each other or multiplied to scalars.
- for a finite-dimensional vector space has an inner product operation we define

as

$$\langle\phi|\psi\rangle = \sum_{k=1}^{d} \phi_k^* \psi_k = \phi_1^*\psi_1 + \phi_2^*\psi_2 + ... = (\phi_1^*, \phi_2^*, ..., \phi_d^*) \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_d \end{pmatrix}, \tag{2.1}$$

where $*$ denotes the complex conjugate, such that the norm is defined by

$$|\psi| = \sqrt{\langle\psi|\psi\rangle}. \tag{2.2}$$

- is conjugate symmetric

$$\langle\psi_1|\psi_2\rangle = \langle\psi_2|\psi_1\rangle^*. \tag{2.3}$$

Let H be the *Hamiltonian*, which in classical mechanics is a function and in quantum mechanics an operator that corresponds to the system's total energy. While this is a trivial statement for the classical version [26]

$$H = \mathrm{T} + \mathrm{V} = E, \tag{2.4}$$

where T denotes the kinetic, V the potential and E the system's total energy, it is less intuitive in quantum mechanics. What we mean when we say that an operator corresponds to a certain observable (a physical quantity which can be measured) is that the operator's eigenvalues correspond to the possible measurement outcomes we can expect when measuring said quantity. The expectation value of the Hamiltonian operator is given by

$$\langle H\rangle_\psi = \langle\psi\,|\,H\,|\,\psi\rangle, \tag{2.5}$$

where $\langle..\rangle$ denotes the average thus $\langle H\rangle_\psi$ corresponds to the system's *average* energy obtained by measuring the observable H of the system in state $|\psi\rangle$ over many repetitions. The Hamiltonian can also be used to obtain and describe a system's time-evolution as we shall see later.

Additionally, we note that while a closed system can mean many things depending on the branch of physics, for this thesis we define a closed system as one that only allows for work exchange between the system itself and the rest of the world, which can be called 'bath','reservoir' or just 'environment'.

Returning to our particle trapped in an infinite square well potential, we point out that if it were in the previously introduced state expressed as vector $|\psi\rangle$, we already could calculate its average energy (2.5). However, something that has not yet been explicitly said is the fact that describing a system with a vector $|\psi\rangle$ implies something about the *knowledge* one has about a given system.

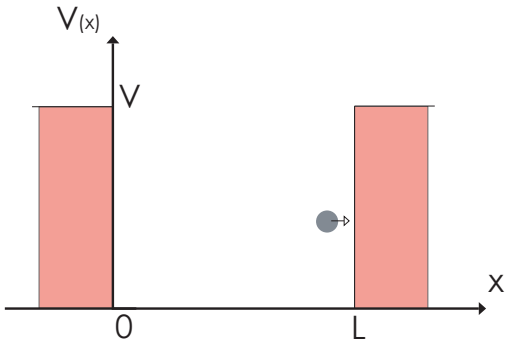


Figure 2.1: Particle trapped in a double well potential

If one has complete information about the state of a quantum system (which may be consist of one or many particles, or may not have a fixed particle number at all), then the system is described by some state vector, as discussed before. Such states are called pure states. However, most often, one only has incomplete information about a quantum system, meaning that one can only give probabilities for finding the system in certain pure states. The system state is then no longer pure, but mixed, and must be described by a density operator (a quantity, which we shall introduce in (2.6)).

We stress here the fact that a single quantum system can be in a mixed state aswell, the amount of states needed to describe a given quantum system is a reflection of the knowledge we have about the system which is maximal for pure states. Since mixed states cannot be described by a single vector we have to use a density matrix, which we define for pure states as

$$\rho = |\psi\rangle\langle\psi| \tag{2.6}$$

and for mixed states as

$$\rho = \sum_i P_i \, |\psi_i\rangle\langle\psi_i| \,, \tag{2.7}$$

where P_i is the probability for an object from the ensemble to be in state $|\psi_i\rangle$.
While for pure states ρ is equivalent to the state vector, the density matrix is a very useful tool when dealing with mixed states because it provides valuable information such as the fact that its n-th entry on the diagonal corresponds to the probability of the system to occupy the quantum state $|n\rangle$. Throughout this thesis we will consider all objects, like the density matrix, to be expressed in the eigenbasis of a system's internal Hamiltonian unless stated otherwise. Additionally, we define its off-diagonal elements as coherences with regard to the specific basis ρ is expressed in.

It is important to point out that while constructing the density matrix of a mixed

state $\{|\psi_i\rangle, P_i\} \rightarrow \rho$, the density matrix is unique. But in the case of a given mixed state ρ it is not possible to uniquely reconstruct the ensemble from which it came $\rho \nrightarrow \{|\psi_i\rangle, P_i\}$, indicating that information has been lost. A few noteworthy properties of ρ are:

$$\text{I.} \quad \text{Tr}(\rho) = 1 \tag{2.8}$$

$$\text{II.} \quad \text{positive semi}-\text{definite } \rho \geq 0 \tag{2.9}$$

$$\text{III.} \quad \text{Pure states } \text{Tr}\left(\rho^2\right) = 1 \tag{2.10}$$

$$\text{IV.} \quad \text{Mixed states } \text{Tr}\left(\rho^2\right) < 1 \tag{2.11}$$

$$\text{V.} \quad \text{Hermitian } \rho^\dagger = \rho \tag{2.12}$$

The term Tr(..) in the equations above denotes the trace over the Hilbert space and † denotes the conjugate transpose. Given a state ρ we define the trace as

$$\text{Tr}(\rho) = \sum_n \langle n|\rho|n\rangle, \tag{2.13}$$

where $\{|n\rangle\}$ is any complete, orthonormal basis.
Additionally, given a state $\rho^\dagger$ we define the conjugate transpose as

$$\rho^\dagger = (\rho^*)^T, \tag{2.14}$$

where T denotes the transpose of a matrix.

Furthermore, let us consider a global system which contains two subsystems, with dimensions d_A, d_B acting on their respective Hilbert spaces $\mathcal{H}_A^{d_A}$ and $\mathcal{H}_B^{d_B}$. Then their global state which acts on $\mathcal{H}_{AB} = \mathcal{H}_A^{d_A} \otimes \mathcal{H}_B^{d_B}$ is given by ρ_{AB}. Given a global state ρ_{AB} one obtains the *reduced* density matrix ρ_A through the partial trace, which we define as

$$\text{Tr}_B(\rho_{AB}) = \sum_{n \in I} \langle n|\rho_{AB}|n\rangle = \rho_A, \tag{2.15}$$

where $I = \{|n\rangle\}_B$ is an orthonormal basis on the Hilbert space $\mathcal{H}_B$. We note that both the definition of global states and partial trace can be expanded for any number of subsystems.

Returning to mixed states, one can see from (2.11) that the *mixedness* which denotes a loss of information, can be estimated by $\text{Tr}(\rho^2) \leq 1$ because the lower $\text{Tr}(\rho^2)$ gets the more mixed the corresponding quantum state is. We define the maximally mixed state then as the state for which $\text{Tr}(\rho^2) = \frac{1}{d}$ where d denotes the dimension of the system.

With this setup at hand let us finally define the average internal energy of said system

$$E(t) = \text{Tr}(\rho(t)H(t)), \tag{2.16}$$

which is easiest to understand when $\rho(t)$ and $H(t)$ are both expressed in the internal Hamiltonian's eigenbasis. In this case the trace is the sum of the probabilities p_i of the system to be in an eigenstate times the corresponding energies ε_i of that eigenstate

$$E(t) = \sum_i p_i \varepsilon_i. \tag{2.17}$$

Additionally, the infinitesimal change in energy $\mathrm{d}E$ can be written as

$$\mathrm{d}E(t) = \mathrm{Tr}(\mathrm{d}\rho(t)H(t)) + \mathrm{Tr}(\rho(t)\mathrm{d}H(t)). \tag{2.18}$$

Thermodynamics considers two modes of energy transfer:

- Work: W is the work done by external parameters, which in this case is captured by the change of the Hamiltonian H.
- Heat: Q is the heat supplied through the interaction with the system's surroundings, which in this case is captured by the change of the density matrix ρ.

Let us now imagine that the potential walls of the square well are pushed towards each other which requires work W, infinitely slowly such that ρ remains unchanged. It is easy to see that in this case $\mathrm{d}W$ is given by

$$\mathrm{d}E = \mathrm{d}W = \mathrm{Tr}(\rho(t)\mathrm{d}H(t)) \tag{2.19}$$

as any change that was done can be be captured by the change of H, such that $\mathrm{Tr}(\mathrm{d}\rho(t)H(t)) = 0$.

Straightforward algebra yields

$$W = -\int_0^\tau \mathrm{Tr}\left(\rho(t)\frac{dH(t)}{dt}\right)dt \tag{2.20}$$

and in similar fashion one obtains for heat

$$Q = \int_0^\tau \mathrm{Tr}\left(\frac{d\rho}{dt}(t)H(t)\right)dt. \tag{2.21}$$

For this thesis we will assume that a positive work value W means that work is being extracted from the system, which is the reason why in this case we have a "-" sign that signals that work is being put into the system unless stated otherwise. For strictly pragmatic reasons we then define a positive heat value Q as heat being absorbed by the system so that a negative value would mean that it is being extracted (from the system). This allows us to easily construct the first law of thermodynamics also called the energy conservation law

$$\Delta E = Q - W. \tag{2.22}$$

The first law of thermodynamic states that any change of a system's internal energy can only be caused through supplying heat or work to the system from an external reservoir or extracting these quantities from the system to a reservoir.

2.2 Second Law of Thermodynamics

The second law of thermodynamics can be formulated in many different ways, but for the purpose of this thesis it is sufficient to define it as a statement about a system's entropy S. To be more exact the second law of thermodynamics states that the total entropy of an isolated system can never decrease as time goes on [11][1]

$$\Delta S \geq 0. \tag{2.23}$$

As has been mentioned, equilibration is a process which is not fully understood for quantum systems. However, Linden et al. were able to show under rather weak assumptions in [12], that for a large evolving quantum system any small subsystem equilibrates towards one state and remains there for almost all times while the large system continues its evolution. Under certain conditions this final state is the 'thermal state' which is of central importance for this thesis and we shall therefore now take a moment to investigate it.

The thermal state is characterized by the fact that it maximizes the entropy for a given energy and is defined as [27]

$$\tau(\beta) = \frac{1}{Z}\exp[-\beta H], \tag{2.24}$$

where we define β as the *coldness* as it is the reciprocal of the system's temperature $\beta = \frac{1}{k_B T}$ [2]. Additionally, Z is known as the partition function and can be seen as normalization, which we define as $Z = \mathrm{Tr}\big(e^{-\beta H}\big)$.

Notice that if we consider $\tau(\beta)$ in the basis of the eigenvectors of the Hamiltonian H it will be diagonal. For a Hamiltonian $H = \mathrm{diag}\{\varepsilon_1, \varepsilon_2, \varepsilon_3, ...\}$ we obtain

$$\tau(\beta)_{ij} = \frac{e^{-\beta\varepsilon_i}}{\sum_{k=1}^{N} e^{-\beta\varepsilon_k}}\delta_{ij}, \tag{2.25}$$

a density matrix whose eigenvalues coincide with the Boltzmann-distribution [11][3] and where δ_{ij} denotes the Dirac delta function [24]. The Boltzmann-distribution

[1] This statement can be found in [11], page 122.

[2] k_B is the Boltzmann constant [11] page 5, which has the value $k_B \approx 1.381 \cdot 10^{-23}$ J/K. From now on we set it to 1 for the remainder of this thesis.

[3] This definition can be found in [11], page 18.

is a probability distribution from statistical mechanics which provides a probability for a system to be in a specific state dependent on the energy and temperature.

Thermal states can be used to define thermal equilibrium because they maximize the entropy for a fixed energy. In the limit $T = 0$ they take the form of pure states, are mixed for $T > 0$ and approach the maximally mixed state for $T \to \infty$.

We stress here the fact that thermal state are of great importance for this thesis and will be re-appearing on many occasions. They carry a number of interesting properties which will be discussed in the following chapters.

Additionally, because the quantum regime is of central interest in this thesis we shall define the von Neumann entropy

$$S_{\mathrm{N}} = -\operatorname{Tr}\Big(\rho \ln(\rho)\Big). \tag{2.26}$$

In mathematical terms the von Neumann entropy is defined as the Shannon entropy of the eigenvalues of ρ, which is used in classical physics to quantify the uncertainty about a classical random variable [11][4]

$$S_{\mathrm{Shannon}} = -\sum_i P_i \log P_i, \tag{2.27}$$

where P_i denotes the probability of outcome i.

Another useful quantity from thermodynamics we will frequently use is the free energy F

$$F = E - TS, \tag{2.28}$$

which is useful to bound the amount of work a system can perform.

Alternatively, in statistical mechanics F can be defined for canonical ensembles, (statistical ensembles that describe possible states for systems at thermal equilibrium) as $F = -k_B T \log(Z)$. Using these definitions and the thermal state from (2.24) the von Neumann entropy (2.26) yields

$$F = \langle E \rangle - T S_{\mathrm{N}}(\tau(\beta)). \tag{2.29}$$

We can see that eq. (2.29) and (2.28) coincide for thermal states.

[4]This definition can be found in [11], page 22.

2.3 Work Extraction in a Closed System

For a better understanding of the recently introduced quantities we shall investigate a closed, d-dimensional quantum system, for which we pick the standard basis to be the eigenbasis of the Hamiltonian (2.30). Again, we stress the fact that a closed system in our context is a system that allows only work exchange between the system and some external work supply through a unitary evolution. We define the system internal Hamiltonian as

$$H_0 = \sum_i^d \varepsilon_i \left|i\right\rangle\!\left\langle i\right|, \varepsilon_i < \varepsilon_{i+1} \tag{2.30}$$

assuming no degeneracy i.e. that every energy value is unique.

We are interested in one of the most fundamental tasks of quantum thermodynamics: extraction and storage of work in quantum systems. In this thesis we shall consider both parts as cyclic Hamiltonian processes which raise (or lower) a system's energy through unitary operations. Even though the exact unitary operations used will differ, depending on the goal of each task, the fundamental principle which governs these processes will remain the same unless stated explicitly otherwise.

Our desire to lower and raise a quantum system's average energy gives rise to concepts such as **passive states** [28] [29], states whose energy cannot be unitarily lowered any further and **maximally activated states** [18], states which have been charged to their maximal capacity and thus their energy cannot be increased unitarily. In this thesis we will deal with work extraction processes first and charging processes later.

To obtain a cyclic Hamiltonian process we consider, in addition to the system's internal Hamiltonian (2.30) an external field $V(t)$, which is turned on at $t = 0$ to extract work from the the system's initial state represented by a density matrix $\rho(0)$. In the presence of the field $V(t)$ the system undergoes a unitary evolution generated by the total Hamiltonian

$$H = H_0 + V(t). \tag{2.31}$$

At the time $t = \tau$ the field $V(t)$ is turned off again returning the system to its initial structure providing cyclicity for the whole process i.e. $H(0) = H(\tau)$.

The system's time evolution is given by the von Neumann-equation [30]

$$\dot{\rho} = -\frac{i}{\hbar}[H_0 + V(t), \rho], \tag{2.32}$$

where $\hbar$ is the reduced Planck constant [11][5] and where $\dot{\rho}$ denotes the time derivative $\dot{\rho} = \frac{d}{dt}\rho$.

The solution of equation (2.32) is given by $\rho(\tau) = U(\tau)\rho U^\dagger(\tau)$ where $U(\tau)$ denotes the overall unitary operator which has been obtained by the time ordered exponent of the generator $H = H_0 + V(t)$

$$U(\tau) = \mathcal{T} \exp\Big(- i \int_0^\tau (H_0 + V(t)dt)\Big), \tag{2.33}$$

where $\mathcal{T}$ denotes the time ordering.

Having control over $V(t)$ in a cyclic Hamiltonian operation such as (2.31) allows us to generate any unitary operation $U = U(\tau)$. This is a very useful property since we will consider only unitary operations on the system in the following.

With this knowledge we can now demonstrate why our assumption that unitary processes only exchange work holds to be true. In (2.21) we have derived a definition of heat

$$Q = \int_0^\tau \mathrm{Tr}\Big(\frac{d\rho}{dt}(t)H(t)\Big)dt, \tag{2.34}$$

where with the use of the time derivation (2.32) we now obtain

$$Q = \int_0^\tau -i \cdot \mathrm{Tr}\Big([H(t), \rho(t)]H(t)\Big)dt = 0 \tag{2.35}$$

with use of the cyclic property of the trace.

Thus, one way to define 'extractable work' is

$$W = \mathrm{Tr}(\rho H_0) - \mathrm{Tr}\big(U\rho U^\dagger H_0\big) \tag{2.36}$$

but as we shall see in chapter 3 there are some issues associated with this approach. Additionally, we point out, that after having argued before that the only variation of the system internal energy comes from $H(t)$ we now know that heat $Q = 0$ for any unitary evolution in a closed system.

Naturally, we would like to know the maximal possible energy gain of any state, which gives rise to *ergotropy* i.e. the maximal extractable work

$$W_{\max} = \mathrm{Tr}(\rho H_0) - \min[\mathrm{Tr}\big(U\rho U^\dagger H_0\big)], \tag{2.37}$$

where $\min[\mathrm{Tr}\big(U\rho U^\dagger H_0\big)]$ denotes the minimal energy state after the evolution.

This is precisely what characterizes the *passive state* [28], which is a state whose

[5]The reduced Planck constant is given by $\hbar = \frac{h}{2\pi}$ where h denotes the Planck constant, $h \approx 6.6 \cdot 10^{-34}$J s. From now on we set $\hbar = 1$ for the remainder of this thesis.

energy cannot be lowered any further by unitary operations. Generally speaking a passive state ρ_p can be written as

$$\rho_p = \sum_i s_i \, |i\rangle\langle i| \tag{2.38}$$

if the values s_i are non-increasing ($s_{i+1} \leq s_i$) for non-decreasing energy eigenvalues $E_{i+1} \geq E_i$ and ρ_p commutes with the system's Hamiltonian H, where $|i\rangle$ denote the eigenstates of the Hamiltonian with eigenvalues E_i and where s_i is the probability for the system to be in a given state $|i\rangle$.

It is important to point out that for every state ρ there is a corresponding passive state ρ_p obtainable through a unitary that arranges the eigenvalues of ρ on the diagonal with respect to the energy eigenbasis in the correct (non-increasing) order. With that the minimal energy $E_{min} = \sum_i \varepsilon_i s_i$ allows us to characterize the ergotropy of ρ as

$$W_{\max} = \mathrm{Tr}(\rho H_0) - \mathrm{Tr}(\rho_p H_0). \tag{2.39}$$

2.4 Complete Passivity and Thermal States

In this chapter we will investigate the fact that when one considers N copies of a passive state

$$\rho_p^{(N)} = \rho_p^{\otimes N}, \tag{2.40}$$

the resulting joint state will generally no longer be passive [6]. Following the analysis of [27] we introduce a quantity called *virtual temperature* β_v which will be assigned to the energy levels of a d-dimensional system ρ with Hamiltonian $H = \sum_n E_n \, |n\rangle\langle n|$. The Hamiltonian H has d energy eigenstates $|i\rangle$ and we assume ρ to be diagonal in the energy eigenbasis $\rho_p = \sum_n s_n \, |n\rangle\langle n|$ given in (2.38).

In general there are $\frac{1}{2}d(d-1)$ different transitions between energy states possible but first we shall consider the transition between $|i\rangle$ and $|j\rangle$. We point out that we neglect any possible degenerate transitions as no work can be extracted by them, hence are of no interest to us. Furthermore, we assume without loss of generality that $i > j$ with which we then define the energy gap as

$$\Delta E_G = E_i - E_j > 0, \tag{2.41}$$

where E_i and E_j are the corresponding energy eigenvalues of states $|i\rangle$ and $|j\rangle$. As has been mentioned before, ρ captures the statistical state of the system by providing the probabilities s_i and s_j for finding the system in the respective eigenstates. For the transition we have introduced in (2.41) the virtual temperature is given by

$$\beta_v = \frac{\log(s_j) - \log(s_i)}{E_i - E_j}. \tag{2.42}$$

Through investigation one will find that β_v will be always *positive* for any passive state (2.38).

We will now consider a second, identical system to the first one, with a different transition $|i'\rangle$ and $|j'\rangle$ with again the corresponding probabilities s'_i and s'_j, an energy gap of same structure as (2.41) $\Delta E'_G = E'_i - E'_j$ and a virtual temperature β'_v defined analogously to (2.42).

The global joint system consisting of both systems allows for some non-trivial transitions. Here we shall focus on the case of transitions between $|i\rangle|i'\rangle$ and $|j\rangle|j'\rangle$. The joint probabilities for the global system to be in these states are given by $s_i s'_i$ and $s_j s'_j$ and we define the joint energy gap as

$$\Delta E_T = E_G + E'_G. \tag{2.43}$$

Using equation (2.42) one obtains

$$\beta_v^{\text{joint}} = \frac{\log(s_j s'_j) - \log(s_i s'_i)}{E_G + E'_G}, \tag{2.44}$$

which can be rewritten as

$$\frac{\log(s_j) - \log(s_i) + \log(s'_j) - \log(s'_i)}{E_G + E'_G} \tag{2.45}$$

and further can be simplified using the definition of the virtual temperature (2.42)

$$\beta_v^{\text{joint}} = \frac{\beta'_v E'_G + \beta_v E_G}{E'_G + E_G}. \tag{2.46}$$

A similar calculation can be done for any non-trivial transition in such a joint system.

Let us now assume that a transition between the levels $|i\rangle$ and $|j\rangle$ with energy gap $E_G = E_i - E_j > 0$ has a negative β_v, which should indicate non-passivity and thus the presence of extractable work W. Considering the unitary transformation

$$U = |i\rangle\langle j| + |j\rangle\langle i| - |i\rangle\langle i| - |j\rangle\langle j| + \mathbb{I}, \tag{2.47}$$

one can obtain the extractable work from (2.36) and will quickly realize that all terms of the trace cancel except for the two energy levels $|i\rangle$ and $|j\rangle$ on which the unitary operator acted

$$W = E_i s_i + E_j s_j - E_i s_j - E_j s_i, \tag{2.48}$$

which can be re-written in the form

$$W = (E_i - E_j)(s_i - s_j) \tag{2.49}$$

$$= (E_i - E_j) s_j (1 - e^{-\beta_v (E_i - E_j)}). \tag{2.50}$$

We know through our assumption that $(E_i - E_j)s_j$ has to be positive and see that $(1 - e^{-\beta_v(E_i - E_j)}) > 0$ for negative values of β_v. So if all terms are positive, W itself has to be positive, showing that work would be extracted from the system undergoing such a transformation thus proving that negative β_v is an indicator of non-passivity.

After establishing the fact that if all possible transitions of a system have a positive β_v it means that there is no unitary transformation which could lower the energy of the system any further, we shall use it to show that systems in specific states remain passive under tensor product, which is also known as being *completely passive* if the virtual temperature has the **same** positive value for all possible transitions.

To demonstrate this, we shall see that if there are multiple copies of the same system present which undergo two (or more) transitions with different β_v, then it will be always possible to find some negative β_v, thus showing non-passivity.

Let us again consider a system in state ρ, with a transition between levels $|i\rangle$ and $|j\rangle$, the energy gap E_G given by (2.41) and virtual temperature β_v. Now let us consider N copies of said system, where the global system undergoes the transition between levels $|i\rangle^{\otimes N}$ and $|j\rangle^{\otimes N}$ with energy gap

$$\Delta E_G^{\text{tot}} = N\Delta E_G \tag{2.51}$$

and the same virtual temperature β_v.

Now let us redo these steps for another K copies undergoing the global transition between the states $|i'\rangle^{\otimes N}$ and $|j'\rangle^{\otimes N}$ with virtual temperature β_v'. The energy gap is given by

$$\Delta E_G'^{\text{tot}} = K\Delta E_G'. \tag{2.52}$$

Just like before the energy gaps are given by $\Delta E_G = E_i - E_j > 0$ and $\Delta E_G' = E_i' - E_j' > 0$. We assume that the corresponding virtual temperatures β_v and β_v' are **different** and additionally related without loss of generality by $\beta_v' > \beta_v$.

We shall now consider the transitions between the states $|i\rangle^{\otimes N}|j'\rangle^{\otimes K}$ and $|j\rangle^{\otimes N}|i'\rangle^{\otimes K}$ of the joint system of $N + K$ copies. The joint transition has the energy gap

$$E_G^{\text{joint}} = N\Delta E_G - K\Delta E_G', \tag{2.53}$$

which can be used to obtain the corresponding virtual temperature

$$\beta_v^{\text{joint}} = \frac{\beta_v N\Delta E_G - \beta_v' K\Delta E_G'}{N\Delta E_G - K\Delta E_G'}, \tag{2.54}$$

where now, through our assumption that $\beta_v' > \beta_v$ we can clearly see that it is always possible to find negative values for the joint virtual temperature β_v^{joint} by choosing the right N and K. More precisely this leads to the condition

$$\frac{E_G'}{E_G} = \frac{N}{K} = \frac{\beta_v' K\Delta E_G'}{\beta_v N\Delta E_G} \tag{2.55}$$

that ensures finding a negative β_v^{joint}.

In doing this we have therefore shown that a joint system with locally passive subsystems, which contain **different** virtual temperatures, no longer necessarily has to be passive itself. By construction one can see that the only way for a state to remain passive under tensor product for any N and K (i.e. be completely passive) is when the virtual temperatures for all possible transitions are positive and identical. As it turns out this condition is only fulfilled for thermal states [27], which we have defined in (2.24) making them the only completely passive states.

2.5 Entanglement and Correlations

Among other things this thesis aims to discuss the relevance of quantum effects such as *entanglement* that can arise when performing extraction and charging protocols in the quantum regime. The following chapter will discuss this physical phenomenon to give the reader a better understanding what it is.

Classical correlations are a concept very familiar to most of us. If one considers two or more physical systems it determines how much knowledge about one system one can gain by measuring some other system. Take the rather simple example of two marbles, one black and one white which are prepared and then sent randomly to two friends Alice and Bob. Alice and Bob know that there are two marbles with different colors but don't know which one is sent to who. Each person on their own has a 50% chance of obtaining either the white or the black marble but as soon as let us say Alice checks the color of her marble and finds out that it is white, she knows with 100% certainty that Bobs marble is going to be black.

To be able to discuss the same scenario in the quantum regime let us consider the pure state

$$\left|\Phi^+\right\rangle = \frac{1}{\sqrt{2}}(|10\rangle + |01\rangle) \tag{2.56}$$

which considers two quantum systems that can be in either states $|0\rangle$ or $|1\rangle$. While the situation here is the same, (someone prepares two particles and sends them to Alice and Bob) there are a few significant differences. First, in the classical case the person preparing the marbles could in theory check which marble is sent to which person. But because of the nature of wave-functions, even the person preparing the particles in state (2.56), is not able to determine which particle is sent to which person. In fact both particles are in neither state until one of them is measured. That would correspond to the marbles not having any color until Alice or Bob would open the package and check. But even if they are in neither state as soon as let us say Alice measures her particle and finds it to be in state $|0\rangle$ she again can say with 100% certainty that Bobs particle will be in state $|1\rangle$. If the particles had no state

prior to Alices measurement how does Bobs particle know which state it has to take?

To answer this question A. Einstein et al. proposed the idea in [31] that each particle, carries hidden variables from the moment of its creation within itself, which, even if unknown to us, determine the outcome of each measurement. The goal was to provide an explanation to this behavior which respects Einsteins postulate that nothing propagates faster than light. Yet through the works of J. S. Bell in [32] it was proven that this proposal is not true. The only assumptions left were either that two particles described through a state as given in (2.56) 'communicate' with each other with no time-delay or that the system's property in question has no definite value *until* it is measured and the outcome is fundamentally random, while still being correlated to the other property of the other system.

This conclusion gave rise to concept of *entanglement* a special type of correlations, which only occur in quantum mechanics.

For pure states which have been introduced in chapter 2.1 a clear distinction can be made between entangled and separable (not entangled states) states of the following form [33]: if the pure global state $|\psi_{AB}\rangle$ can't be written as tensor product of the pure states corresponding to its subsystems

$$|\psi_{AB}\rangle \neq |\psi_A\rangle \otimes |\psi_B\rangle \tag{2.57}$$

it is said to be *entangled*. If that is the case the subsystems can no longer be accurately described as single entities without taking the other one into consideration. On the other hand, if it can be rewritten in such a fashion then it would be called *separable* and no entanglement is present. Additionally, if one were to consider an N-partite pure state which can only be written as a tensor product of maximally L-terms, it is said to be L-separable [15].

Just like with classical correlations, entanglement in a global system increases the more additional information the global state ρ_{AB} has when compared to the information we have about A and B individually [34]. A quantity used to capture this relation is the mutual information [24]

$$I(\rho_A, \rho_B) = S(\rho_A) + S(\rho_B) - S(\rho_{AB}), \tag{2.58}$$

where in the quantum regime the von Neumann entropy defined in (2.26) is used for S.

Equation (2.58) shows that correlations or entanglement increase with our decrease in knowledge (increase in entropy) of the local parts A and B and reach its maximum when A and B are maximally mixed i.e. no predictions can be made about the local outcomes of the single sub-systems which is exactly the case for the state (2.56).

The maximal value reachable for $I(\rho_A, \rho_B)$ is given by [35]

$$I(\rho_A, \rho_B) = \log(d) \quad \text{for separable states and} \tag{2.59}$$

$$I(\rho_A, \rho_B) = 2\log(d) \quad \text{for entangled states,} \tag{2.60}$$

where d denotes the dimension of the system showing that entanglement represents a especially strong type of correlations.

Additionally, we point out that mutual information defined in (2.58) can be used as entanglement measure for global pure states in the sense that the global entropy for them is per definition always $S(\rho_{AB}) = 0$. Hence $I(\rho_A, \rho_B)$ is only non-zero for entangled states, for which the local entropies $S(\rho_A)$ and $S(\rho_B)$ are non-zero.

This, however, is no longer the case for mixed states for which it is significantly harder to distinguish between correlations and entanglement. Hence there the mutual information just measures correlations and can not be used for entanglement in general. For additional reading on the topic of correlations in mixed states see [36].

Chapter 3

Work Fluctuations

Something that has not been properly addressed yet is the fact that we are considering thermodynamic quantities such as work on the quantum scale where thermal and quantum fluctuations become prevalent. Because of this fact work must be treated as a random variable of stochastic nature, which means that its possible values are determined by the outcomes of a random process.

Additionally, because the dynamics of such small systems are heavily influenced by fluctuations, the second law of thermodynamics has to be generalized for the non-equilibrium regime. These are the goals of the *fluctuation theorems* [37],[38],[39] we shall consider in this chapter.

Explained in simple terms fluctuation theorems (FTs) deal with classical, isolated systems whose Hamiltonian's parameters are changed in a time interval $[0, \tau]$ in order to drive its initial, thermal state out of equilibrium. For this scenario the work performed on the system is a randomly distributed quantity W. Thus, repeating this process many times will provide us different work values, from which one can calculate the average work $\langle W \rangle$.

Another helpful quantity which we will use is the free energy difference between the initial and final equilibrium states given by

$$\Delta F = -\beta^{-1} \ln \frac{Z_{H_\tau}}{Z_{H_0}}, \tag{3.1}$$

where Z_t denotes the corresponding canonical partition function with Hamiltonian H_t. We stress here the fact that after the process which drives the system out of equilibrium discussed above results in a non-equilibrium final state. The quantity given in (3.1) denotes the difference of free energies between the initial equilibrium state and a final equilibrium state into which the system would relax after the process, if it had the time [40].

The first generalization of the second law of thermodynamics for systems which are arbitrarily far from equilibrium, has been done by D. J. Evans et al. in [41].

Since for small systems, fluctuations play a significant role, thermodynamic quantities such as work acquire a stochastic nature which results in the fact that the second law has to be expressed using probability distributions. The conclusion in [41] was that processes which generate negative entropy are exponentially more rare than their positive entropy generating counterparts. This statement shows that a generalization of the second law is still valid for small systems that have been driven out of equilibrium.

We point out that the Jarzynski-equation which will be discussed in the next section, represents a more accessible approach to characterize work fluctuations. This is the reason why much has been done [8][42][7] to be able to find an analogue of it in the quantum regime, where coherence can be present. The main problem of this task is the fact that in the quantum regime, as has been mentioned, a clear definition of what exactly constitutes work is hard.

Because work characterizes a process, it cannot be associated with a specific state of a system in quantum mechanics, consequently it cannot be described by Hermitean operators. Thus, the classical approach to define work as the difference of two points in the phase-space is no longer possible in quantum mechanics [9].

That is why the most commonly used definition of work in the quantum regime is the 'two projective measurement scheme' [9], which defines the work as the difference of two measurement outcomes. But as we will see in 3.4 this approach fails to characterize work for coherent processes, which is why we will discuss other theoretical approaches at the end of this chapter. Ultimately we will prove in 3.5 that our trouble of defining work properly does not come from a lack of knowledge but is of fundamental nature.

3.1 Classical Jarzynski and Crooks

To properly understand the issue, let us consider the classical Jarzynski equality [37], which allows one to make a connection between equilibrium free energy difference defined in ΔF 3.1 to the non-equilibrium work defined through measurements. By doing so, it provides a generalization of the second law of thermodynamics into the non-equilibrium regime.

Let us consider a classical, thermally isolated system initially in thermal equilibrium (2.24) on which work W is to be performed by changing a work parameter λ of the system with Hamiltonian $H(\lambda)$ in the time interval $[0, \tau]$. After time τ has passed we let the system thermalize again to a new equilibrium state. If one would change λ infinitely slowly between initial point A and final point B such that the system would have enough time to equilibrate at any point along the path γ so that it effectively stays in equilibrium at all times, the process would be isothermal (which means that the temperature remains constant) and thus we can define the

work performed on the system to be equal to the difference in the Helmholtz Free energy [11][1]

$$W = \Delta F = F^B - F^A, \tag{3.2}$$

where F^A and F^B are the free energies corresponding to the initial thermal state before and final equilibrium state after work W has been performed and we let the system thermalize. In this chapter we shall consider a positive W to correspond to the work put into the system to drive it out of equilibrium.

Now let us consider the same process with the alteration that λ now gets changed at a finite rate such that the system is brought out of equilibrium. Jarzynski was able to show in [37] that for the stochastic definition of work in thermally isolated systems equation

$$\langle e^{-\beta W} \rangle = e^{-\beta \Delta F} \tag{3.3}$$

holds. Applying Jensen's inequality, which states that $e^{\langle x \rangle} \leq \langle e^x \rangle$ simple algebra yields

$$\langle W \rangle \geq \Delta F. \tag{3.4}$$

Both equations hold for all time intervals $[0, \tau]$. Note that the system started initially in a equilibrium state but the final state can be arbitrarily far away from equilibrium. Also we point out that even though we have restricted ourselves to a very simplistic case, the relations established are fairly general and can be shown to hold even for cases where coupling between the system and environment is present [43].

In this sense, equation (3.3) is able to make a connection between the non-equilibrium work performed on the system and the equilibrium free energy difference ΔF. Additionally, equation (3.4) is a statement about the fact that the average work in this scenario will be always larger than the work necessary for the quasi-static process (3.2), which is a known consequence of the second law of thermodynamics. Thus, the Jarzynski equality represents a generalization of the second law of thermodynamics into the non-equilibrium regime.

Two years after the introduction of the Jarzynski-equation (3.3) Gavin Crooks using the principle of micro-reversibility established in [38] a more generalized version of it known as the 'Crooks fluctuation theorem'

$$\frac{P(W, \lambda)}{P(-W, \tilde{\lambda})} = e^{\beta(W - \Delta F)}, \tag{3.5}$$

[1] This definition can be found in [11], page 25.

where $P(W, \lambda)$ denotes the probability density function, which describes the probability to find an energy consuming process while $P(-W, \tilde{\lambda})$ denotes the probability of finding the corresponding energy releasing process and $\tilde{\lambda}$ denotes the time reversed parametrization, which relates to λ through $\lambda_{\tau-t} = \tilde{\lambda}_t$.

G. Crooks defined $P(-W, \tilde{\lambda})$ as the time reversed process, which in this context means that for every trajectory $z(t)$ between initial point A and final point B there is a backwards protocol that can invert the direction of time and run the trajectory backwards. For further information read [8].

Let us consider once again the quasi-static case of $W = \Delta F$. Immediately we see that (3.5) reduces to

$$P(W, \lambda) = P(-W, \tilde{\lambda}) \tag{3.6}$$

in which case the probabilities for both, energy consuming and their corresponding energy releasing processes are equal. Both probabilities being equally likely implies a reversible process ($\Delta S = 0$,$Q \to 0$) from which we know that it obeys the first law of thermodynamics

$$\Delta E = W. \tag{3.7}$$

Simultaneously the limit case $\Delta F = 0$ of equation (3.5), shows the very fundamental feature that energy consuming processes are exponentially more likely than their energy releasing counterparts, which is just another way to phrase the second law of thermodynamics.

3.2 Quantum Approach

As we just have seen the Jarzynski equation is able to provide us with information such as a lower bound for $\langle W \rangle$ by ΔF from (3.4) for these protocols. Additionally, it gives us more exact statements about the second law of thermodynamics and allows us to extract equilibrium information from a non-equilibrium quantity.

An interesting question that naturally follows is whether one can find an analogue of the Jarzynski relation in the quantum domain. A major obstacle of this task is the fact that a clear definition of work is hard in the quantum regime. In the following sections we shall discuss different approaches scientists have taken to resolve this issue and recover the desired relations from classical physics.

3.3 Work operators

The first attempts were made by Bochkov and Kuzovlev in [21] and afterwards a more generalized approach by Yukawa in [44] where they defined work equivalently to the classical case as the difference between the initial and final Hamiltonians. But since the Hamiltonians correspond now to operators work itself is defined as an operator $\mathcal{W}$ in the Heisenberg picture

$$\mathcal{W} = H_\tau^H - H^H, \tag{3.8}$$

where the superscript H indicates the Heisenberg picture in which operators are time-dependent and are defined as

$$H^H(t) = U^\dagger(t) H U(t) \tag{3.9}$$

in which U denotes the time evolution operator (time propagator).
As such the work $\mathcal{W}$ performed on or by the system can be always be identified with an average energy change of the system for all initial states.

But at the same time [21] was not able to provide a quantum analogue to the Jarzynski-equation (3.3) for the work operator $\mathcal{W}$ in the paper, which is a necessary condition to properly characterize work. The conclusion of this paper states that quantum processes might not have a valid definition of work.

As we shall see later, even though this prediction holds partially true, P. Talkner and P. Hänggi were able to show in [45] that the base assumption that work could be described by an operator is wrong. They point out that work characterizes a process rather than a state of a system and as such cannot be described by any Hermitian matrix, whose eigenvalues can be determined by a single projective measurement.

3.4 Two Projective Measurement Scheme

One of the most established ways to describe work fluctuations is the two projective measurement scheme (TPMs) introduced by P. Talkner et al. in [9]. As the name indicates it consists of two projective measurements of which the first is performed at the beginning and the second at the end of the process. An important feature of the TPM is the fact that it is able to generalize the Jarzynski equality (3.3) into the quantum regime and capture the process-dependent nature of work W itself.

But despite its many advantages the projective measurements are very invasive processes that destroy any coherence the system had prior to them [46][47]. So

while being able to characterize work fluctuations the TPM scheme is only able to do so for classical initial states, which means that it is not able to study the thermodynamics of coherent processes. Even if new coherence would arise between the first and second measurement, the fact that *at* the measurements coherence is lost prevents quantum interference effects, which are a central tool in quantum physics.

Let us now consider the specifics of the TPM scheme. First we prepare a thermally isolated quantum system in equilibrium, which can be described via density matrix

$$\rho = \sum_i P_i \left|\psi_i\right\rangle\!\left\langle\psi_i\right|, \tag{3.10}$$

where P_i are the corresponding probabilities to the different states $|\psi_i\rangle$ of the System.

Then work is performed on the system by externally varying the Hamiltonian of ρ such that the evolution

$$\rho \to \rho_f \tag{3.11}$$

can be described by a unitary matrix U, such that $\rho_f = U\rho U^\dagger$ and

$$H \to H_f. \tag{3.12}$$

In this case the initial and final Hamiltonian can be represented in the their respective energy-eigenbasis as follows:

$$H = \sum_n E_n \left|n\right\rangle\!\left\langle n\right|, \tag{3.13}$$

$$H_f = \sum_m E_{m,f} \left|m_f\right\rangle\!\left\langle m_f\right| = \sum_m E_{m,f} V \left|m\right\rangle\!\left\langle m\right| V^\dagger, \tag{3.14}$$

where $E_n, (E_{m,f})$ denotes the corresponding initial (final) energy of state $|n\rangle$ ($|m_f\rangle$) and V a unitary operator that transforms the Hamiltonian basis such that

$$\left|m_f\right\rangle = V \left|m\right\rangle. \tag{3.15}$$

Let us assume the first projective measurement at the beginning of the process measures energy E_n with probability $P_n = \langle n \,|\, \rho \,|\, n\rangle = \rho_{nn}$, after which the system evolves according to the protocol and the second measurement at the end obtains the energy value $E_{m,f}$. Here we are interested in the conditional probability of obtaining $E_{m,f}$ given we already measured E_n in the past

$$P_{n,m} = \left|\left\langle m_f \,|\, U \,|\, n\right\rangle\right|^2 = \left|\left\langle m \,|\, V^\dagger U \,|\, n\right\rangle\right|^2. \tag{3.16}$$

With E_n and $E_{m,f}$ at hand the TPM scheme allows us to define the work that has been performed on the system as

$$W_{(nm)} = E_n - E_{m,f} \tag{3.17}$$

with the respective probability

$$P_{(nm)} = P_{n,m}\rho_{nn}, \tag{3.18}$$

that denotes the probability of finding an evolution for a given W.
In the case of degeneracies i.e. more than one evolution for the same work value the whole probability distribution can be written down as

$$P(W) = \sum_{nm} \delta(W - W_{(nm)})P_{(nm)}. \tag{3.19}$$

This result can be used to determine the average work according to the TPM scheme

$$\langle W \rangle^{\mathrm{TPM}} = \sum_{W} P(W)W \tag{3.20}$$

as the energy difference of the initial and final states as we defined them

$$\sum_{W} P(W)W = \sum_{n} E_n\rho_{nn} - \sum_{n,m} E_{m,f}p_{(nm)}. \tag{3.21}$$

Using (3.16), the fact that for any complete set of states $|l\rangle$ we know $\sum_l |l\rangle\langle l| = \mathbb{I}$ and the relation

$$V^{\dagger}_{nm} = V^{*}_{mn}, \tag{3.22}$$

where the asterisk $*$ denotes the complex conjugation, (3.21) can be rewritten as

$$\begin{aligned}\sum_{n} E_n\rho_{nn} - \sum_{n,m} E_{m,f}p_{(nm)} &= \sum_{n} E_n\rho_{nn} - \sum_{n,m} E_{m,f}\rho_{nn}\,|\langle m\,|\,V^{\dagger}U\,|\,n\rangle|^2 \\ &= \sum_{n} E_n\rho_{nn} - \sum_{n,m} E_{m,f}\rho_{nn}\langle n\,|\,U^{\dagger}V\,|\,m\rangle\langle m\,|\,V^{\dagger}U\,|\,n\rangle,\end{aligned} \tag{3.23}$$

which then using equation (3.20) yields

$$\langle W \rangle^{\mathrm{TPM}} = \sum_{n} E_n\rho_{nn} - \sum_{n,m} E_{m,f}\rho_{nn}U_{ln}U^{*}_{kn}V_{km}V^{*}_{lm}. \tag{3.24}$$

At the same time since the evolution is unitary, no heat is generated (as has been previously argued, $Q = 0$), which means that because of the first law of thermodynamics (2.22) the performed (or extracted) work alone is responsible for the change of the system's average energy during such a process thus

$$\begin{aligned}\langle W \rangle = \Delta E &= \mathrm{Tr}\big(\rho H^i\big) - \mathrm{Tr}\big(U\rho U^{\dagger}H^f\big) \\ &= \sum_{n} E_n\rho_{nn} - \sum_{i} \langle i|\,U\rho U^{\dagger}H^f\,|i\rangle \\ &= \sum_{n} E_n\rho_{nn} - \sum \langle i|\,U\rho U^{\dagger}E_{m,f}V\,|m\rangle\langle m|\,V^{\dagger}\,|i\rangle\end{aligned}$$

$$= \sum_n E_n \rho_{nn} - \sum E_{m,f} \rho_{nj} U_{ln} U^*_{kj} V_{km} V^*_{lm}. \tag{3.25}$$

Comparison of (3.24) and (3.25) shows that both definitions agree only with each other if index $j = n$, i.e. if the initial states have only diagonal entries and thus are classical.

This just reiterates what has already been mentioned, that while the TPM scheme is able to reproduce our classical findings such as the first law of thermodynamics $\langle W \rangle = \Delta E$ in the quantum regime, it does so only for classical states. This finding led researchers to look for other measurement schemes that could both generalize fluctuation theorems into the quantum regime and conserve coherence simultaneously.

Additionally, we point out that the measurements considered in the TPM scheme are idealized. This means that the measurement device (pointer) and the system in question are perfectly correlated before the measurement such that by 'observing' the pointer one can conclude the state the system is in with probability 1. However, Y. Guryanova, N. Friis and M. Huber show in [48] that such perfect correlations require an infinite supply of resources, thus while representing helpful tools for theorists are not realizable in practice.

3.5 POVMs and No-Go Result

The main obstacles regarding the problem of work characterization in the quantum regime can be boiled down to two conditions which we will now investigate. M. Perarnau-Llobet et al. argue in [22] that within quantum theory there is no fluctuation theorem that can

1. Respect that work relates to average energy change for all initial states

$$\sum_W P(W) W = \mathrm{Tr}\big(\rho H^i\big) - \mathrm{Tr}\big(U \rho U^\dagger H^f\big). \tag{3.26}$$

2. Reproduce the results of the TPM scheme for classical initial states.

In order to prove that the inability to find a scheme that fulfills both necessary conditions is of fundamental nature, we shall use the most generalized quantum measurements, represented by positive operator-valued measures (POVMs). A POVM is a set of operators $\{M^{(W)}\}$ that satisfy

$$M^{(W)} \geq 0 \text{ and } \sum_W M^{(W)} = 1. \tag{3.27}$$

As one can see every work value has its own associated operator $M^{(W)}$ that can be used to determine the work probability distribution

$$P(W) = \mathrm{Tr}\big(\rho M^{(W)}\big) \tag{3.28}$$

and thus we define the average work of a certain process as

$$\langle W \rangle = \sum_W \mathrm{Tr}\big(\rho M^{(W)}\big) W. \tag{3.29}$$

By introducing a new operator

$$X = \sum_W W M^{(W)} \tag{3.30}$$

the average work can be expressed as

$$\langle W \rangle = \mathrm{Tr}(X\rho), \tag{3.31}$$

which together with condition 1 (3.26) can be rewritten such that

$$\langle W \rangle = \mathrm{Tr}(X\rho) = \mathrm{Tr}\big(\rho H^i\big) - \mathrm{Tr}\big(U\rho U^\dagger H^f\big). \tag{3.32}$$

From the cyclic property of the trace it follows

$$X = H^i - U^\dagger H^f U. \tag{3.33}$$

Now with the proper tools at hand it is worth mentioning that in [49] it was recently shown that the TPM scheme can also be described by such POVMs and be written as

$$M_{\mathrm{TPM}}^{(nm)} = \sum_{nm} \delta(W - W_{(nm)}) p_{n,m_f} \left|n\right\rangle\!\left\langle n\right|, \forall \rho = D(\rho), \tag{3.34}$$

where D is a dephasing operation that removes all coherence. This allows us to express condition 2 for all POVMs as

$$\mathrm{Tr}\big(\rho M^{(W)}\big)) = \mathrm{Tr}\Big(\rho M_{\mathrm{TPM}}^{(nm)}\Big). \tag{3.35}$$

Following [22] in which M. Perarnau-Llobet et al. showcased that there is no scenario where X can satisfy both (3.33), which is equivalent with condition 1 and (3.34) that represents condition 2 simultaneously.

For better understanding let us imagine a single two-level system with initial and final Hamiltonians $H^i = \varepsilon \left|1\right\rangle\!\left\langle 1\right|$, $H^f = \tilde{\varepsilon} \left|1\right\rangle\!\left\langle 1\right|$ that undergo a unitary evolution $U = \left|0\right\rangle\!\left\langle +\right| + \left|1\right\rangle\!\left\langle -\right|$, where $\left|\pm\right\rangle = \frac{1}{\sqrt{(2)}}(\left|0\right\rangle \pm \left|1\right\rangle)$.

Starting with (3.33) straightforward calculation yields $X_{(1)} = \varepsilon \left|1\right\rangle\!\left\langle 1\right| - \tilde{\varepsilon} \left|-\right\rangle\!\left\langle -\right|$.

At the same time (3.34) reduces in the non-degenerate case to $M^{(nm)} = p_{n,m_f} |n\rangle\langle n|$. With (3.16), our newly defined X (3.30) reduces for this specific U to

$$X = \frac{1}{2} \sum_{nm} W_{(nm)} |n\rangle\langle n| \tag{3.36}$$

and thus results in $X_{(2)} = -\frac{\tilde{\varepsilon}}{2} |0\rangle\langle 0| + \frac{2\varepsilon - \tilde{\varepsilon}}{2} |1\rangle\langle 1|$ which obviously contradicts the result we got for $X_{(1)}$. This fact leads to the conclusion that any possible measurement scheme that reproduces classical results for classical initial states will disturb the whole process such that the average energy will be changed destroying the energy-work relation from condition 1.

3.6 Quasi-Probabilities

While for some the no-go theorem discussed in the previous section demonstrates a limit, M. Lostaglio proposed in [20] a way to circumvent it by considering a family of protocols that smoothly interpolate between the TPM scheme giving us $P_{nm} = P_{\text{TPM}}$ and a protocol from [7] yielding a work probability distributions P_{weak} obtained by weak measurements. Weak measurements represent a class of measurements which, in contrast to the 'strong', idealized measurements considered in the TPM scheme, couple the pointer to the system very weakly [50] [51], which leads to errors as one cannot infer with complete certainty the state of the system by 'observing' the pointer. Thus, additionally post-selection is necessary to discard the undesired outcomes.

To obtain P_{weak} the protocol in [7] probes quasi-probabilities, which can be negative and as such have no clear physical meaning.

Now let us investigate the specific steps of the interpolation protocol:

1. We consider an initially uncorrelated measurement device, which we represent as a 1-dimensional quantum system in a Gaussian state with spread s

$$|\psi\rangle = (\pi s^2)^{1/4} \int dx \exp[-x^2/(2s^2)] \, |x\rangle \, , \tag{3.37}$$

   which represents a superposition of different position eigenstates. Thus, the eigenstates of the position operator, are weighted by a Gaussian distribution.

2. We start by correlating our system ρ with the pointer in the time interval $[-\tau, 0]$ through an interaction Hamiltonian H_i.

3. After the coupling process is completed at $t = 0$ we perform a weak projective measurement on the pointer by setting $s \to \infty$ which induces a POVM on the system ρ and yields energy E_n.

4. After the first measurement has been completed, we let the system evolve (similarly to the TPM scheme) unitarily in the time interval $[0, \tau]$.

5. Finally at $t = \tau$ a strong, projective measurement is performed from which we obtain result E_{m_f}.

To show that this interpolation protocol is a generalization of the TPM scheme let us consider two important limits. Let P_{m_f} be the probability to obtain energy E_{m_f} from the second measurement and let $\langle X \rangle_{m_f}$ be the expectation value of the shift in the pointer after the second measurement.

In the limit of $s \to 0$ the induced POVM on the system ρ from step 3 approaches a strong, projective measurement such that

$$P_{m_f} \langle X \rangle_{m_f} \to P_{(nm)} = P_{n,m} \rho_{nn} \tag{3.38}$$

takes the form of the TPM scheme (3.18).

While in the proposed limit of $s \to \infty$ we obtain a weak measurement such that

$$P_{m_f} \langle X \rangle_{m_f} \to P_{\text{weak}} = \operatorname{Re} \operatorname{Tr}\big(\rho \varepsilon_n \Pi_{m_f}\big), \tag{3.39}$$

where $\varepsilon_n = |n\rangle\langle n|$ and $\Pi_{m_f} = U^\dagger |m_f\rangle\langle m_f| U$. Notice that we are considering only the real part of the trace in (3.39) because it can turn negative for certain choices of ρ. A negative probability has no clear physical interpretation.

The distribution obtained by P_{weak} corresponds to the quasi work distribution introduced in [7] known as the Margenau-Hill distribution [52].

Because $P_{(nm)}$ and P_{weak} are both obtained by the same family of protocols the interpolation protocol has to be a FT protocol i.e. it fulfills condition 2 from chapter 3.5 and is able to reproduce the TPM scheme for classical, initial states. But additionally in the weak measurement limit $s \to \infty$ it is also able to fulfill condition 1 and respect the fact that work relates to an average energy change for all initial states. The corresponding fluctuation theorem is then [7]

$$\langle e^{-\beta W} \rangle = e^{-\beta \Delta F} \Upsilon, \tag{3.40}$$

where $\Upsilon = \operatorname{Re} \operatorname{Tr}\big(U^\dagger \gamma(\tau) U \gamma(0)^{-1} \rho\big)$ and where $\gamma(t) = e^{-\beta H(t)} / \operatorname{Tr}\big(e^{(-\beta H(t))}\big)$. We can clearly see that in the case of $\rho = \gamma(0)$ we get $\Upsilon = 1$, which just reduces the equation to the standard Jarzynski equation (3.3).

As we have seen this protocol allows to fulfill both conditions simultaneously but does so only with the addition of unphysical negative probabilities. This leads to the conclusion that every approach we have considered, ultimately failed to satisfy both conditions 1, 2 and to be measurable at the same time. Each of them has some advantages but suffers from different drawbacks that cannot be overcome. For comparison see table 3.1.

	Measurable	Coherent Proc.	Fluct theory
Operator of Work	✓	✓	x
TPM scheme	✓	x	✓
Quasiprobabilities	x	✓	✓

Figure 3.1: Comparison between the three discussed approaches to characterize work fluctuations in the quantum regime: The operator of work 3.3, the TPM scheme 3.4 and Quasi-probabilities 3.6. Each approach fails to satisfy all necessary conditions, which further confirms the no-go result obtained in 3.5.

3.7 Outlook

Additionally, it is worth being mentioned that M. Perarnau-Llobet argued in [53] that while it is not possible for any measurement scheme to fulfill conditions 1 and 2 simultaneously **and** be measurable, significant advantages can be gained by performing global measurements on multiple copies of the system instead of using single measurements on one system. This approach reduces the back action of the measurement apparatus drastically, thus while not being able to completely characterize work fluctuations for quantum processes, is at least able to give a better description of them.

Chapter 4

Quantum Batteries

Batteries are omnipresent in our daily lives. Regardless of whether we are talking about small cells in computers or calculators, which have capacities as low as 100 miliwatt-hours or consider energy storage systems used in vehicles, which reach capacities up to 500 kilowatt-hours, batteries play an indispensable role in modern society [54]. However, the miniaturization of technology requires us to consider batteries on increasingly small scales, where eventually thermal and quantum fluctuations become non-negligible.

This undertaking gives rise to the concept introduced by R. Alicki and M. Fannes, called *quantum batteries* (QBs)[19], small quantum mechanical systems which can be used to temporarily store energy for later use. We shall describe QBs as either infinite or d-dimensional systems, with non-degenerate energy levels whose thermodynamic role is to act as a reservoir for work.

Since on a fundamental level engines perform their tasks based on repeated cycles during which the systems dynamics are changed through some external control we will apply the same approach for quantum batteries. This means considering the cyclic, time-dependent Hamiltonian introduced in (2.31) to describe the system's evolution.

Actually the d-dimensional quantum system in section 2.3 could be labeled as quantum battery since it meets all the requirements, which we shall revise here.

First, we note that the battery's initial state depends on the exact goal of the protocol in question. For the charging processes discussed in 4.4, whose goal it is to increase the average energy of the battery, it makes sense for us to consider the QB to be initially in an 'empty', thermal state, because we have argued in 2.4 that it is the only passive state which remains passive under tensor product. However, for the work extraction protocols we investigate, whose goal it is to lower the systems average energy, it is sufficient to consider the QB to be initially in a non-passive state from which work can be extracted through unitary operations. A single system is

non-passive if condition (2.38) is not fulfilled. However, as we know from section 2.4 a multipartite system consisting of locally passive subsystems does not have to be globally passive. It will only remain passive under tensor product if it's subsystems are copies of the same thermal state.[1]

Second, we consider ideal reversible processes to extract (or charge) energy from (into) a QB. These processes are controlled by the internal Hamiltonian H_0, that captures the system's dynamics and an external time dependent field $V(t)$, which is turned on for a time-period $[0, \tau]$.

Additionally, since the processes we are considering take place in the quantum regime, we shall study whether quantum effects such as entanglement can occur and if they do how they influence the dynamics of the process.

First we will focus on work extraction protocols and eventually in section 4.3 we will start to investigate specific charging protocols.

4.1 Work Extraction in the Context of Multiple Batteries

Let us quickly revise the main points of the work extraction chapter 2.3:

- A single quantum battery with internal Hamiltonian H_0 is considered to be initially in a non-passive state $\rho = \rho(0)$, which we consider in the energy eigenbasis.

- To extract work, an externally controlled field $V(t)$ is applied, which causes the system to undergo a time evolution described by the von Neumann equation $\dot{\rho} = -i[H_0 + V(t), \rho]$.

- The maximal extractable work from a QB during such a process is given by the ergotropy defined in (2.37) $W_{\max} = \mathrm{Tr}(\rho H_0) - \mathrm{Tr}(\rho_p H_0)$, where ρ_p is the corresponding passive state to ρ.

[1] For completeness this argument can be extended taking β into consideration. A global state consisting only of subsystems in the thermal states (2.24) $\tau(\beta_1)$ and $\tau(\beta_2)$ is only passive iff $\beta_1 = \beta_2$. Thus, we shall assume identical β when considering multipartite ensembles $\tau(\beta)^{\otimes N}$, for the remainder of this thesis unless stated otherwise.

Following the analysis of [19] we shall now consider how extractable work behaves in the presence of multiple identical copies of the battery. We remember the thermal state (also known as canonical Gibbs state) from (2.24) at inverse temperature β

$$\tau(\beta) = \frac{1}{Z}\exp[-\beta H], \tag{4.1}$$

where $Z = \mathrm{Tr}\big(e^{-\beta H}\big)$ and the von Neumann entropy (2.26)

$$S_{\mathrm{N}} = -\,\mathrm{Tr}\Big(\rho \cdot \ln(\rho)\Big). \tag{4.2}$$

For every density matrix ρ a specific inverse temperature β_s can be found for which $S(\rho) = S(\tau(\beta))$. Using the condition of stability of thermodynamics, which asserts that thermal states, which maximize the entropy for a given energy, minimize the free energy defined in (2.28) [55][2] we obtain

$$\mathrm{Tr}(\rho H_0) - \frac{1}{\beta_s}S(\rho) \geq \mathrm{Tr}(\tau(\beta)H_0) - \frac{1}{\beta_s}S(\tau(\beta)). \tag{4.3}$$

From this we conclude that

$$\mathrm{Tr}(\rho H_0) \geq \mathrm{Tr}(\rho_p H_0) \geq \mathrm{Tr}(\tau(\beta)H_0) \tag{4.4}$$

which sets a bound for the maximal extractable work $W_{\max}$

$$W_{\max} \leq \mathrm{Tr}(\rho H_0) - \mathrm{Tr}(\tau(\beta)H_0). \tag{4.5}$$

Now we shall take N copies of the battery and observe how the maximal extractable work behaves for each independent battery. For this we need to consider the joint system's Hamiltonian

$$H_0^{(N)} = H_0 \otimes .... \otimes 1 + ... + 1 \otimes .... \otimes H_0 \tag{4.6}$$

that can be used to define the maximal extractable work **per copy**

$$w_{\max}^N = \frac{1}{N}\left[\mathrm{Tr}\Big(\big(\rho^{(N)}H_0^{(N)}\big) - \mathrm{Tr}\Big(\rho_p^{(N)}H_0^{(N)}\Big)\Big)\right], \tag{4.7}$$

where $w_{\max}^N$ is the extractable work per copy of the joint system. Additionally, $\rho^{(N)} = \rho^{\otimes N}$ denotes the joint N-partite density matrix and $\rho_p^{(N)}$ is the joint passive state, consisting of individual passive states ρ_p, that correspond to their respective states ρ.

Here we note that it was shown in chapter 2.4 that while all thermal states are passive not all passive states are thermal. Considering multiple joint passive states $\rho_p^{(N)}$ as we just have seen in (4.7), leads to the so called *activation* [27], where in the case of a composite system that consists of multiple passive states, the corresponding density matrix $\rho_p^{(N)}$ may contain population inversion [56] and as such allow for

[2]This relation can be found in [55], page 42.

work extraction.

R. Alcki and M. Fannes were able to show in [19], that with increasing number of copies N the average energy per copy of the passive state $\rho_p^{(N)}$ decreases (see figure: 4.1). A decrease in energy of the passive state is associated with an increased $w_{\max}^N$ and thus an increase of extractable work of the total system has been achieved.

As it turns out this additional extractable work is only accessible for entangling unitaries that act globally on all N copies simultaneously. This shows that while a quantum advantage is possible for work extraction when compared to their classical counterparts, global unitaries might create entanglement. This is undesirable because entanglement, or more generally correlations have been shown to signal extractable work [14][57][58]. From this we infer that if the final global state, after the entangling unitary, has been applied contains correlations, it is in fact not passive.

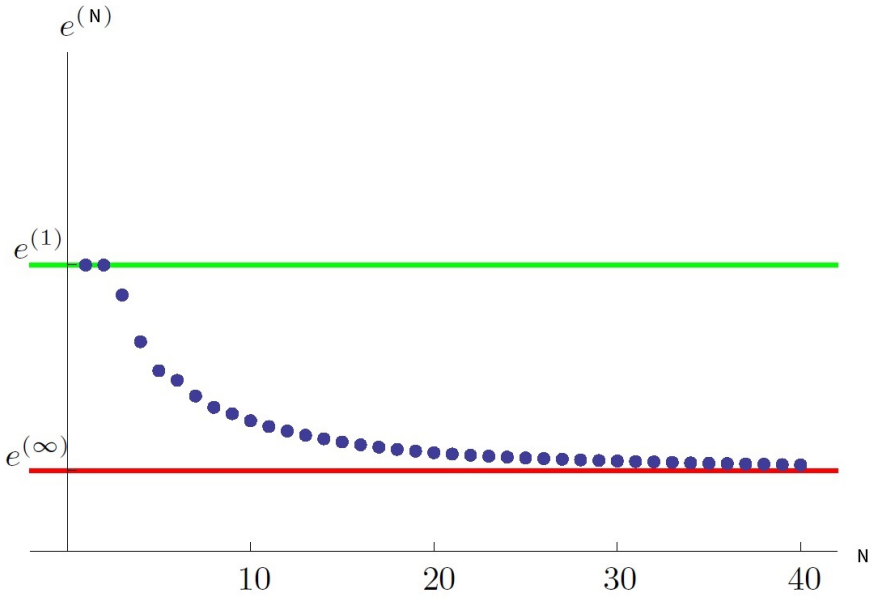


Figure 4.1: The energy **per copy** $e^{(N)}$ of the joint passive state $\rho_p^{(N)}$, which was obtained from the joint intial state $\rho^{(N)}$, plotted for $N = 1, ..., 40$ identical copies. The additional extractable work, accessible only for global unitaries for any N, is quantified by the difference between $e^{(1)}$ and $e^{(N)}$. Notice that the maximal additional extractable energy obtained, in the case $e^{(\infty)}$ is bounded as discussed in eq. (4.8). This graphic has been taken from [19], page 2.

Furthermore, the authors were able to provide a bound to the additional extractable work when considering $\rho_p^{(N)}$. In fact for the limit $N \to \infty$ one obtains [19]

$$\lim_{N\to\infty} w_{\max}^N = \frac{1}{N}\left[\mathrm{Tr}\Big(\big(\rho^{(N)}H_0^{(N)}\big) - \mathrm{Tr}\Big(\rho_p^{(N)}H_0^{(N)}\Big)\Big)\right] = \mathrm{Tr}(\rho H_0) - \mathrm{Tr}(\tau(\beta)H_0). \tag{4.8}$$

As we just have seen global entangling unitaries, that act simultaneously on all

individual systems, are necessary to maximize the possible work gain from multiple batteries. In the next chapter we shall investigate this behavior in more detail.

4.2 Avoidable Entanglement

As has been mentioned previously in chapter 4.1, there seems to be a connection between the entanglement generated by global unitaries and the maximal extractable work from multipartite systems. The claim made there was that global unitaries are able to extract more work from a set of quantum systems, when compared to local unitaries, each acting on one specific system. We will later see that using such entangling unitaries does not automatically imply that entanglement has to be always created. Using a specific protocol allows us to avoid entanglement generation but it comes at a cost: it takes more time lowering the *power* of the work extraction process.

Following the works of K. Hovhannisyan et al. in [15], we shall see that using the entangling operator to make a *direct* exchange of two diagonal entries of a density matrix, i.e. the typical fast way will always lead to at least some entanglement generation.

For this task we shall consider N identical, non-interacting, non-passive finite-dimensional quantum systems

$$\rho^{\otimes N} = \rho^{(N)}. \tag{4.9}$$

We consider each system with the Hamiltonian we already introduced $H_0 = \sum_i \varepsilon_i \, |i\rangle\langle i|$ with $\varepsilon_i < \varepsilon_{i+1}$, which composes the Hamiltonian of the total ensemble

$$H_0^{(N)} = H_0 \otimes .... \otimes 1 + ... + 1 \otimes .... \otimes H_0 \tag{4.10}$$

whose eigenbasis we shall use as standard basis.

Additionally, we consider the system to be in a product state made of the corresponding locally passive states, which are passive but not thermal and are diagonal in the total Hamiltonian $\rho_p^{(N)}$ where $\rho_p = \mathrm{diag}\{p_1, p_2, ..., p_d\}$ with $p_i \geq p_{i+1}$ and $\sum_i p_i = 1$ as defined in (2.38).

We point out that the way we construct $\rho_p^{(N)}$, it is by definition a fully separable state. Now analogously to previous chapters an external field $V(t)$ is used to extract energy from the joint system. And again a global entangling operator which acts on all subsystems simultaneously, is used. As has been shown in (4.8), the operator which maximizes the extracted work, is the one that aligns the elements such that they're not increasing, i.e. such that the final state is a globally passive state. Even though the resulting final state is separable, the fact that we are using

non-local unitaries might lead to entanglement creation during the process [59].

Let us assume that all we need to do to achieve the joint passive state is the exchange of the populations P_n by P_m, whose corresponding eigenstates are $|n\rangle = |i_1^n i_2^n ....i_N^n\rangle$ and $|m\rangle = |i_1^m i_2^m ....i_N^m\rangle$.

A generic unitary able to exchange two such basis states as $|n\rangle$ and $|m\rangle$ is defined as

$$U^{nm} = \sum_{\mu \neq n,m} |\mu\rangle \langle\mu| + |n\rangle\langle m| + |m\rangle\langle n| \quad \text{where} \quad n \neq m. \tag{4.11}$$

If we control the external field $V(t)$, which generates the unitary (4.11) to such a degree that we can make sure it couples only to the states $|n\rangle$ and $|m\rangle$, then the evolution operator at any given moment t of the process is defined as [15]

$$U^{nm}(t) = \sum_{\mu \neq n,m} |\mu\rangle\langle\mu| + u^{nm}(t), \tag{4.12}$$

where $u^{nm}(t)$ denotes a unitary that operates on the linear span of $|n\rangle$ and $|m\rangle$ and depends on t and $V(t)$.

Additionally, we point out that it is generally a more challenging task to quantify entanglement generated in a multipartite systems, than in the case of two systems as discussed in chapter 2.5. In said chapter we have argued that once the subsystems of a composite system in a pure state are mixed it indicates entanglement. This property can be applied similarly for bigger systems by considering the reduced matrix

$$\rho_{12} = \mathrm{Tr}_{3,4,\ldots,N}\left(\rho_p^{(N)}\right), \tag{4.13}$$

where $\mathrm{Tr}_{3,4,\ldots,N}$ is the partial trace defined in (2.15). If all bipartite partitions obtained this way have mixed reduced density matrices then the state $\rho_p^{(N)}$ is genuinely N-partite entangled [60][61].

We point out that this conclusion can only be made about pure composite systems and thus was presented purely for didactic purposes. K. Hovhannisyan et al. used [15] a measure of genuine multipartite entanglement for mixed states [19][62], which can be applied for the states we are considering.

Returning to the exchange between the populations P_n and P_m we know from equation (4.8) that the resulting final energy will correspond to the energy of a thermal state

$$\lim_{N\to\infty} W \to N\,\mathrm{Tr}\Big[\Big(\rho_p - \tau(\beta)\Big)H_0\Big] \tag{4.14}$$

in the thermodynamic limit.

With the use of the fact that the global entropy is invariant under unitaries, the definition for the thermal state (2.24) and the property $\mathrm{Tr}(\rho_p - \tau(\beta)) = 0$ (4.14) yields

$$N\Big[\mathrm{Tr}(\rho\log\rho) - \mathrm{Tr}(\rho\log\tau(\beta))\Big] = N \cdot TS(\rho_p||\tau(\beta)), \tag{4.15}$$

where $S(||)$ is the relative entropy [63] used to quantify the distinguishability between two states, which in quantum mechanics acts as a measure of entanglement [64].

To gain more insight let us now consider a direct exchange of the two basic states $|n\rangle$ and $|m\rangle$ with corresponding populations $P_n = \prod_{j=1}^{N} P_{i_j^n}$ and $P_m = \prod_{j=1}^{N} P_{i_j^m}$.

To demonstrate what these populations correspond to, imagine the eigenstate of the total Hamiltonian $H_0^{(2)}$ defined in (4.10) for two systems ($N = 2$) $|n\rangle = |i_1^n i_2^n\rangle = |0_1^n\, 0_2^n\rangle$ where $|0_1^n\rangle$ and $|0_2^n\rangle$ are eigenstates of the Hamiltonians $H_{0,1}$,$H_{0,2}$ of the respective locally passive subsystems $\rho_{p,1}$, $\rho_{p,2}$. Now $P_{i_1^n}$ is the population of the eigenstate $|i_1^n\rangle$ of the first subsystem H_1, which is the first element of the eigenstate $|n\rangle$ of the total Hamiltonian $H_0^{(N)}$.

For such an exchange we obtain [15]

$$E_k \geq |P_n - P_m| - 2k\sqrt{P_n P_m}, \tag{4.16}$$

where the value of E_k is the k-th entry of an ordered string that is called *entropy vector*, where $E_1 \geq E_2 \geq ..... \geq E_{2^{N-1}-1}$.

The entropy vector can be used to quantify correlations or entanglement present in a given state, after a transposition in the following way: If the last $2^{L-1} - 1$ entries of this vector are 0, then the state as a whole is L-separable, which means for pure states that the state vector can be expressed as tensor product of L terms 2.5. This brings us to two main conclusions:

- In the case of all entries being 0, it would mean that the state is N-separable thus no entanglement is present. But just the first $E_1 \geq 0$ is enough to conclude that there is some entanglement.

- If no entries are 0, it means 1-separability for the state or in other words genuine N-partite entanglement, which can be measured by looking at the smallest value of the entropy vector $E_{2^{N-1}-1}$.

With some algebra in the case of $P_n \geq P_m$ we know the state to be (at most) L-separable if the following condition is fulfilled

$$\frac{P_n}{P_m} \geq 1 + 2\gamma + 2\sqrt{\gamma + \gamma^2}, \tag{4.17}$$

where

$$\gamma = 2^{N-1} - 2^L + 1. \tag{4.18}$$

Furthermore K. Hovhannisyan et al. were able to show that (4.17) implies the condition

$$S(\tau(\beta)||\rho_p) \geq \frac{1}{N}\ln\left[1 + 2\gamma + 2\sqrt{\gamma + \gamma^2}\right], \tag{4.19}$$

which the state ρ_p has to fulfill to be (at most) L-separable during the transposition process in question.

Condition (4.19) can be interpreted as a statement, that as the difference between $\tau(\beta)$ and ρ_p grows, qualitatively more entanglement will be generated during the extraction process. At the same time we know that the extractable work W depends on the difference between $\tau(\beta)$ and ρ_p as well. So the bigger the difference, the more work can be extracted but also the more entanglement will be generated during the process. This leads to the conclusion that there is a relation between extractable work W and generated entanglement.

Additionally, it is worth pointing out that the condition for *any* entanglement to be present $S(\tau(\beta)||\rho_p) \geq \ln(3 + 2\sqrt{2})/N$ is much easier fulfilled for $N \gg 1$ than the condition for genuine N-partite entanglement $S(\tau(\beta)||\rho_p) \geq \ln(2)$.

K. Hovhannisyan et al. then proceeded in [15] to show that it is possible to achieve the same inversion **without** generating any entanglement if one were to break the transposition process down into $2N-1$ 'smaller' population exchanges that yield the same result. If we assume that every transposition requires the same finite amount of time this would mean that we can use entangling operators to maximize the extractable work from an ensemble, without generating any actual entanglement at the cost of losing power

$$\langle P \rangle = \frac{W}{\tau}, \tag{4.20}$$

where $\langle P \rangle$ denotes the average power during the work extraction process and τ is the time necessary to achieve the desired final state, given that the process started at $t = 0$.

Now let us look at the specifics of how exactly it is possible to avoid entanglement generation during the process. As we remember, work extraction is possible if two (or more) populations P_n and P_m violate condition $p_i \geq p_{i+1}$ and can be re-ordered. This re-ordering can be done in one 'fast' process i.e. exchanging the population P_n by P_m directly or alternatively in multiple exchanges that yield the same result. As has been already mentioned, breaking the process down into $2N-1$ steps allows us to avoid entanglement, while reaching the same desired final state in which all populations are ordered non-increasingly.

To exchange the populations P_n by P_m we need to consider the corresponding eigenstates $|n\rangle = |i_1^n i_2^n ....i_N^n\rangle$ and $|m\rangle = |i_1^m i_2^m ....i_N^m\rangle$ of the total Hamiltonian $H_0^{(N)}$. The $2N-1$ exchanges can be broken down into two phases:

- Phase 1: Using the unitary defined previously in (4.11), the first entry of $|n\rangle$, i_1^n is exchanged with the first entry of $|m\rangle$, i_1^m, where $|i_1^n\rangle$ and $|i_1^m\rangle$ correspond to eigenstates of the first subsystem's Hamiltonian H_1 such that

$$|i_1^n i_2^n ....i_N^n\rangle \Leftrightarrow |i_1^m i_2^n ....i_N^n\rangle \,. \tag{4.21}$$

  This process is done N-times (in total) until

$$|i_1^m i_2^n ....i_N^n\rangle \Leftrightarrow |i_1^m i_2^m ....i_N^n\rangle \Leftrightarrow .... \Leftrightarrow |i_1^m i_2^m ....i_N^m\rangle \,. \tag{4.22}$$

  While this sequence achieves that population P_n reaches the desired position, it does so at the cost of neglecting P_m and bringing many other populations of the states in the chain of permutations out of order. Hence a second phase is necessary to bring P_m into the desired position and all the other populations back into their original places.

- Phase 2: After phase 1 has been performed, we take the state $|i_1^m i_2^m ....i_N^{\mathbf{n}}\rangle$ and do the same process backwards

$$|i_1^m i_2^m ....i_N^n\rangle \Leftrightarrow ... \Leftrightarrow |i_1^m i_2^n ....i_N^n\rangle \Leftrightarrow |i_1^n i_2^n ....i_N^n\rangle \tag{4.23}$$

  until we reach $|n\rangle$ after $N-1$ steps. After phase 2 has concluded P_n and P_m have been exchanged while all other entries are back in their original place.

This sequence of steps allows us to reach the desired final, globally passive state without generating any entanglement. It is worth pointing out that these exchanges happen only for global states for which all other entries remain fixed except for the two which are exchanged. For example in the first step of phase 1 the exchange between $|i_1^n\rangle$ and $|i_1^m\rangle$ takes only place if all other entries $|i_2^n, i_3^n, ...i_N^n\rangle$ are fixed. We point out that it is possible in general, that some eigenstates $\left|i_j^n\right\rangle$, $\left|i_j^m\right\rangle$, where j denotes the subspace the eigenstates correspond to, can coincide lowering the amount of necessary steps.

Now let us again consider the unitary (4.11) for these transpositions. As has been shown, the operator can be written for any moment t of the process as

$$U^{nm}(t) = \sum_{\mu \neq n,m} |\mu\rangle\langle\mu| + u^{nm}(t). \tag{4.24}$$

But if we now consider the specific unitary $U^{n,n'}$ that is required to make the step

$$|n\rangle = |i_1^n i_2^n ....i_N^n\rangle \Leftrightarrow |i_1^m i_2^n ....i_N^n\rangle = |n'\rangle \,, \tag{4.25}$$

we can express the operator according to (4.24) at any moment t as

$$\rho^{(N)}(t) = U^{n,n'}\rho^{(N)}(0)U^{n,n'\dagger}$$

$$= (P_n + P_{n'})\rho_1(t) \otimes |i_2^n....i_N^n\rangle\langle i_2^n....i_N^n| + \sum_{\mu\neq n,n'} P_\mu\,|\mu\rangle\langle\mu| \tag{4.26}$$

with $\rho_1(t) \geq 0$ and $\mathrm{Tr}(\rho_1(t)) = 1$. From (4.26) one can see that even though $U^{n,n'}$ is a global operator, the subspace corresponding to the first battery remained separable during the entire transposition process $|n\rangle \Leftrightarrow |n'\rangle$, which then is equivalently valid for any of the following $2N$ transpositions. As we have discussed in chapter 2.5 a separable state is per definition not entangled.

In this chapter we have seen that entangling operators allow us to extract work that local operators don't have access to. Additionally, we have seen that while entangling operators are necessary to maximize the extractable work in multipartite systems, entanglement per se is not. It is when we start to also maximize the power of the work extraction process that entanglement starts playing a role.

4.3 Charging Quantum Batteries

After having discussed the details of how work extraction can be performed and what quantum effects one can expect to encounter, we shall now consider the second major topic of this thesis: **battery charging**. We will consider the same cyclic Hamiltonian processes introduced in chapter 2.3 to perform this task. The goal of the charging process discussed in this section will be to increase the average energy while additionally maximizing the power we define in (4.27). Finally, in section 4.4, we will consider a charging process which minimizes the charging precision in detail.

Here we will follow the analysis of F. C. Binder et al.[18], where we shall focus on charging any initial state ρ to a final state ρ^f, where $\mathrm{Tr}(\rho H) < \mathrm{Tr}\big(\rho^f H\big)$. As such the exact initial and final states ρ and ρ^f are not relevant to us as long as they meet our requirement. Instead we shall focus on maximizing the power during the charging process

$$\langle P\rangle = \frac{\langle W\rangle}{\tau}, \tag{4.27}$$

where τ is the process duration.

Just like in chapter 2.3, we consider a charging process in which the initial state ρ undergoes a unitary, cyclic evolution for time τ generated by the Hamiltonian

$$H(t) = H_0 + V(t), \tag{4.28}$$

where $V(t)$ has only non-zero values in the time interval $[0, \tau]$.

However, since we are interested in maximizing the charging power (4.27) this time τ is not an arbitrary value but instead part of the optimal solution because as we shall see the charging rate $\frac{d}{dt}E(\rho)$ is a time-dependent function.

Before we discuss the driving protocol in detail, a few additional points have to be made because τ is now a relevant variable:

- 1. We consider our evolution to be cyclic because sudden quenches where in the limit of the duration τ approaching 0, the power approaches infinity for finite amounts of work such that

$$\lim_{\tau \to 0} P \to \infty. \tag{4.29}$$

- 2. One could still argue that it is possible to charge the battery via the cyclic evolution infinitely fast such that again $\tau \to 0$. This is prevented by the quantum speed limits (QSL) [65][66], which pose a fundamental bound as to how fast such evolutions can be. It is important to point out that these limits do **not** represent the most optimal charging times i.e. the processes with the lowest τ are not necessarily the most efficient in terms of charging power.

- 3. In order to simulate realistic scenarios we restrict the amount of energy available for the driving process by restricting the trace norm $||H(t)|| \leq E_{\max}$, where we define the trace norm as

$$||H|| = \mathrm{Tr}\Big(\sqrt{HH^\dagger}\Big), \tag{4.30}$$

  and $\dagger$ is the conjugate transpose defined in (2.14).

After having laid out the foundations, let us consider the details of charging a single qubit optimally - that is, optimizing eq.(4.27). We define the system's internal Hamiltonian which describes a two-state system as $H_0 = |1\rangle\langle 1|$. We shall parametrize the total Hamiltonian with control functions $v^x(t)$,$v^y(t)$ and $v^z(t)$ for Pauli operators σ^x, σ^y and σ^z such that

$$V(t) = v^x(t)\sigma^x + v^y(t)\sigma^y + v^z(t)\sigma^z = \begin{bmatrix} v^z(t) & v^x(t) - iv^y(t) \\ v^x(t) + iv^y(t) & -v^z(t) \end{bmatrix}, \tag{4.31}$$

where one can see that the instantaneous eigenvalues of $V(t)$ are
$\lambda^{\pm} = \pm\sqrt{(v^x(t))^2 + (v^y(t))^2 + (v^x(t))^2}$. We can group the control functions $v(t) = (v^x(t), v^y(t), v^z(t))^T$ and Pauli operators $\sigma = (\sigma_x, \sigma_y, \sigma_z)^T$ such that $V(t) = v(t) \cdot \sigma$. Additionally, we shall add the following constraint to the maximal difference between the eigenvalues λ^+ and λ^-

$$\lambda^+ - \lambda^- \leq E_{\max} \ \forall\, t \tag{4.32}$$

and since we are using unitary transformations we know that the state's global purity is conserved. Considering the protocol in the Bloch picture allows us to parametrize ρ with the angles θ and ϕ and the radius r. Because of the purity constraint we know r has to remain constant during the whole process, while, as we shall see later, the angle ϕ has no relevance for the optimal power charging protocol, i.e. we only care about the z-coordinate on the Bloch-sphere.

In order to optimize the average work done during the driving process we shall again consider the von Neumann time evolution (2.32), which can be re-written with the Pauli operators

$$i\frac{d}{dt}\rho(t) = [H_0 + V(t), \rho(t)] = \frac{1}{2}[v(t)\cdot\sigma, \mathbb{I} + a(t)\cdot\sigma], \tag{4.33}$$

where $a(t)$, called the bloch vector of ρ, represents the Cartesian coordinates in terms of the Pauli operators by which $\rho(t)$ is parametrized

$$a(t) = \begin{bmatrix} a^x(t) \\ a^y(t) \\ a^z(t) \end{bmatrix} = r \begin{bmatrix} \sin\theta(t)\cos\phi(t) \\ \sin\theta(t)\sin\phi(t) \\ \cos\theta(t) \end{bmatrix}. \tag{4.34}$$

The solution of (4.33), which is given by

$$\rho(t) = \begin{bmatrix} a^x(t)v^y(t) - a^y(t)v^x(t) & A + iB \\ A - iB & a^y(t)v^x(t) - a^x(t)v^y(t) \end{bmatrix}, \tag{4.35}$$

where $A = a^y(t)v^z(t) - a^z(t)v^y(t)$ and $B = a^x(t)v^z(t) - a^z(t)v^x(t)$ and can be rewritten using the Einstein summation convention as

$$\frac{d}{dt}\rho(t) = v^j(t)a^k(t)\varepsilon_{jkl}\sigma^l, \tag{4.36}$$

where ε_{jkl} is the Levi-Civita symbol, which equals to 1 if (j,k,l) are even permutations of $(1,2,3)$, or equals -1 if (j,k,l) are odd permutations of $(1,2,3)$ and finally 0 if any index is repeated.

As has been said, the goal of the protocol is to increase the average energy of the system with respect to the internal Hamiltonian H_0, optimally. To achieve that, we shall first find the optimal solution for $\frac{d}{dt}E = \frac{d}{dt}\operatorname{Tr}(\rho H_0)$ for each moment t during the process for $0 \leq t \leq \tau$. After that, we shall calculate the optimal duration τ to have the complete solution.

Let us start by finding the optimal solution for $\frac{d}{dt}\operatorname{Tr}(\rho H_0)$, which using equation (4.35), can be rewritten as

$$\operatorname{Tr}\left(\frac{d}{dt}\rho(t)H_0\right) = a^x(t)v^y(t) - a^y(t)v^x(t)$$

$$= r\sin\theta(t)\cdot\Big(v^y(t)\cos\phi(t) - v^x(t)\sin\phi(t)\Big). \tag{4.37}$$

The optimal solution for equation 4.37 has been found for $v^x(t) = -E_{\max} \sin\phi(t)$, $v^y(t) = E_{\max} \cos\phi(t)$ and $v^z(t) = 0$ [18] such that

$$\mathrm{Tr}\left(\frac{d}{dt}\rho(t)H_0\right)_{\text{optimal}} = r \sin\theta(t) E_{\max}, \tag{4.38}$$

where $E_{\max}$ is the angular speed of $\theta(t) = \theta_0 + E_{\max}t$.
On the Bloch sphere the solution corresponds to a geodesic with constant r and because of $v^z(t) = 0$ we can determine that there is no driving in the direction of the reference Hamiltonian H_0.

Now after having found the optimal solution for $\frac{d}{dt}\mathrm{Tr}(\rho H_0)$, it is time to optimize the power for any initial state ρ_i

$$\langle P \rangle = \frac{\langle W \rangle}{\tau} = \frac{\mathrm{Tr}(\rho_f H_0) - \mathrm{Tr}(\rho_i H_0)}{\tau}, \tag{4.39}$$

which using the result from (4.38), equation (4.39) can be rewritten as

$$\begin{aligned} &\frac{E_{\max}}{\theta_\tau - \theta_0}\ r\ \left(\frac{\cos\theta_0 - \cos\theta_\tau}{2}\right) \\ &\qquad = \frac{r}{2\tau}(\cos\theta_0 - \cos\theta_\tau). \end{aligned} \tag{4.40}$$

The solution for the optimal charging time τ_{opt} is found by solving

$$\cos\theta_{\tau_{\text{opt}}} - E_{\max}\tau_{\text{opt}}\ \sin\theta_{\tau_{\text{opt}}} = \cos\theta_0. \tag{4.41}$$

After having found the parameters which maximize the charging power for a single qubit evolution, we will now consider joint systems $\rho^{(N)} = \rho^{\otimes N}$ as seen in 4.2, whose joint reference Hamiltonian (again) is the sum of the local Hamiltonians defined in (4.10). Here we note that Binder et al. added the condition of *no degradation* [18] by considering only unitaries which don't decrease the purity of the local subsystems. This has been done because optimization over all possible unitary transformations is not analytically feasible. Additionally, since the goal of [18] is to show that global entangling operations can achieve an advantage in terms of power per qubit when compared to the single qubit case we have just discussed, Binder et al. concluded that it is sufficient to show said advantage for one specific global evolution.

For simplicity we will restrict our calculations to N pure states on which we perform charging $|0\rangle^{\otimes N} \to |1\rangle^{\otimes N}$ to demonstrate an advantage in terms of power per qubit when compared to charging a single battery. Let us first consider the Hamiltonian for charging each qubit parallel, locally [18]

$$H^{(N)}_{0,\text{par}} = E_{\max}(\cos\phi_0\sigma_x - \sin\phi_0\sigma_y) \otimes \mathbb{I} \otimes ... + ... + ...\mathbb{I} \otimes E_{\max}(\cos\phi_0\sigma_x - \sin\phi_0\sigma_y), \tag{4.42}$$

which has equally distributed $N + 1$ eigenvalues and the difference between the biggest and smallest eigenvalue is $NE_{\max}$. In order to have a fair comparison we

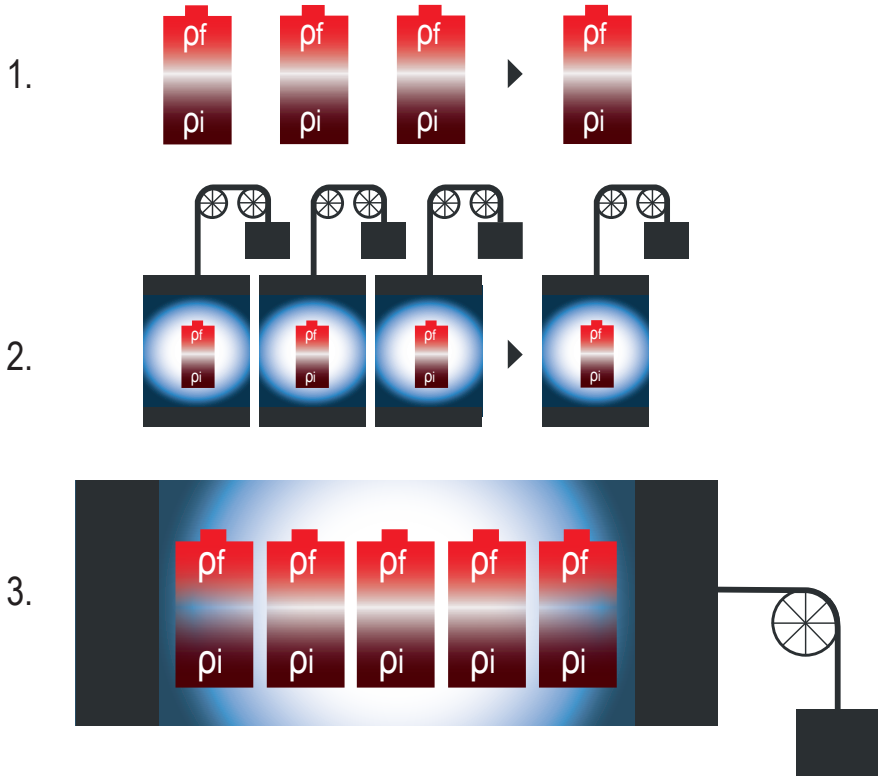


Figure 4.2: Consider an ensemble of qubits acting as quantum batteries (1) with initial (uncharged) and final (charged) states ρ_i and ρ_f, which can be either charged parallel by local operations (2) or globally (3).

shall assume that the Hamiltonian corresponding to the entangling process has the same difference between the biggest and smallest eigenvalues $E_{\max}^{(N)} = NE_{\max}$.

If we assume for simplicity that the average work per qubit during the full charging process is unity we obtain the total work performed on the system to be $\langle W \rangle = N$ which allows us to calculate the optimal time for the parallel charging process

$$\tau_{\text{opt,par}} = \pi(E_{\max})^{-1}. \tag{4.43}$$

Now let us consider the case where we use global entangling operations to fully charge the batteries. By repeating the same calculations as above but instead with the joint Hamiltonian

$$H_{0,\text{glo}}^{(N)} = E_{\max}^{(N)}\Big(\sigma_x \otimes \mathbb{I} \otimes ... + ... + ... \otimes \mathbb{I} \otimes \sigma_x\Big) \tag{4.44}$$

this time, we obtain the optimal time for the global charging process $\tau_{\text{opt,glo}} = \pi(E_{\max}^{(N)})^{-1}$.

$$\tau_{\text{opt,glo}} = \pi(E_{\max}^{(N)})^{-1}. \tag{4.45}$$

Using both solutions in (4.27) we clearly see that

$$\langle P_{\text{par}} \rangle N = \langle P_{\text{glo}} \rangle \tag{4.46}$$

i.e. a N-fold advantage, in terms of power per qubit has been reached by allowing global operations.

Additionally, worth pointing out is the fact that while global entangling operations reach an N-fold advantage the initial and final state remain separable. F. C. Binder et al. [18] argue that while during the charging process entanglement is created, it starts to decrease towards the end as seen in Fig.4.3 until the final state $|1\rangle^{\otimes N}$ is completely disentangled. A more intricate analysis regarding the consequences and limits of this quantum advantage is discussed by F.Campaioli et al. in [67].

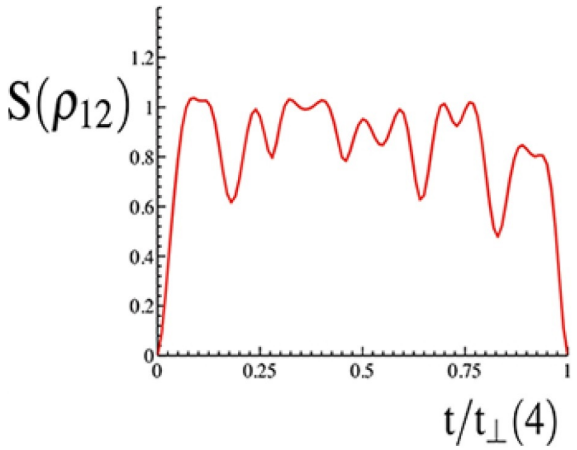


Figure 4.3: The entopies behavior during the global charging process plotted for four qubits. The reduced state ρ_{12} has been obtained by tracing over the last two qubits using the partial trace defined in (2.15). Note that the initial and final states have vanishing entropies which indicate disentanglement. This graphic has been taken from [18], page 9.

4.4 Fluctuations and Precision during Battery Charging

After having discussed the advantage of power one obtains by allowing global entangling unitaries for charging multiple quantum batteries in section 4.3 we point out that unitaries that charge a quantum battery by a fixed amount are **not** unique. This means that one can consider other properties of the battery during the charging process than the charging power.

The goal of this chapter is to follow the analysis of N. Friis and M. Huber in [1] where the authors consider charging ensembles of harmonic oscillators via the same cyclic Hamiltonian processes introduced in 2.3. These ensembles, which act as initially empty batteries, are going to be charged by a fixed amount ΔE through different unitaries to compare the behavior of the following two quantities

- 1. The **charging precision**, quantified by the variance V, is an important quantity because just knowing the final average charge is not all that one might be interested in. It is crucial to consider the individual final energy deviations from the average energy, to ensure that one is sufficiently likely to obtain the desired charge in a measurement. Thus, a low variance indicates that most of the final energies will be close to the expected average energy [11]. For charging a thermal state we define the charging precision to be the change of the standard deviation of the system's Hamiltonian

$$\Delta\sigma = \sqrt{V(\rho_f)} - \sqrt{V(\tau(\beta))}, \tag{4.47}$$

  where $\tau(\beta)$ denotes the initial thermal state introduced in (2.24), ρ_f the final (charged) state and where $V(\rho)$ which denotes the system's energy variance is given by

$$V(\rho) = (\Delta H(\rho))^2 = \mathrm{Tr}\big(\rho H^2\big) - (\mathrm{Tr}(\rho H))^2. \tag{4.48}$$

- 2. The **work fluctuations** during the charging process capture the average square deviations of the necessary work W for different iterations of the charging process from the average energy ΔE. We define the work fluctuations as

$$(\Delta W)^2 = \sum_{n,m} P_{(nm)}(W_{(nm)} - \langle W\rangle)^2, \tag{4.49}$$

  where $P_{(nm)}$,$W_{(nm)}$ are defined in the TPM scheme chapter (3.17). Additionally, we recall that for the TPM scheme the condition $\Delta E = W$ holds for initially classical states. Thus, we obtain for initial thermal states $\tau(\beta)$

$$(\Delta W)^2 = \sum_{n,m} P_{(nm)}(W_{(nm)} - \Delta E)^2. \tag{4.50}$$

Considering infinite-dimensional systems such as harmonic oscillators with (angular) frequency ω and constant energy gap ω will allow us to study the behavior of these quantities at each instant in specific charging protocols. Thus, we define the system's Hamiltonian as

$$H_0 = \sum_n^{\infty} n\omega \ |n\rangle\langle n|, \tag{4.51}$$

where ω is the oscillator frequency and where the corresponding thermal state $\tau(\beta)$ is then

$$\tau(\beta) = (1 - e^{-\beta\omega}) \sum_{n=0} e^{-n\beta\omega} \ |n\rangle\langle n| \ . \tag{4.52}$$

Choosing the thermal state as our initial state guarantees not only that the battery is empty (in the sense that no more work can be extracted from it i.e. passive) but also that it will remain empty, as has been argued, in chapter 2.4, should we ever consider multiple batteries in thermal states at once.

Finally we will consider d-dimensional systems with finite d, with the same constant energy gaps to obtain new results which are not contained in [1] in section (4.5).

4.4.1 Precision and Fluctuation Limits at Zero Temperature

For clarity let us look at the simple case of charging one single battery, which is initially in thermal equilibrium at temperature $T = 0$ (in units of ω) [3]. The corresponding density matrix is then given by $\tau = |0\rangle\langle 0|$ and the system's Hamiltonian is given by (4.51). Additionally, in this specific case the charging precision and work fluctuations coincide such that [1]

$$(\Delta W)^2 = (\Delta\sigma)^2 = V(\rho_f), \tag{4.53}$$

where ρ_f is the final (charged) state given by $\rho_f = U \ |0\rangle\langle 0| \ U^\dagger = |\psi\rangle \ \langle\psi|$. This gives us the opportunity to simultaneously cover the bounds of one quantity by exploring the bounds of the other.

Here we will focus on the charging precision where we will investigate the fact that as long as we assume the system's Hilbert space to be infinite-dimensional, $(\Delta\sigma)^2$ is **not** upper bounded.

To clarify further, let us consider that we want to charge the battery by a fixed amount ΔE. This task can be achieved in many ways but there is nothing from

[3] The temperature is given in units $\frac{\hbar\omega}{k_B}$, but since we have set $\hbar = k_B = 1$ it will be given in units of ω for the remainder of this thesis.

stopping us from considering a superposition of $|\psi\rangle = \sqrt{p}\,|0\rangle + \sqrt{(1-p)}\,|k\rangle$, where p can be chosen in such a way that we achieve the desired final energy for any sufficiently large k. It is true that with increasing k the corresponding probability $\sqrt{(1-p)}$ decreases, but if we chose to define $k = (1-p)^{-1}\Delta\epsilon$ where $\Delta\epsilon = \frac{\Delta E}{\omega}$ we obtain for the charging precision

$$\left(\frac{\Delta\sigma_{\text{worst}}}{\omega}\right)^2 = \Delta\epsilon(\, k - \Delta\epsilon), \tag{4.54}$$

where one can clearly see that the charging precision does not depend on $\sqrt{(1-p)}$. This in turn allows us to make the probability arbitrarily small, thus increasing k as we see fit for a fixed ΔE. This means that in the worst case charging a battery just by a small amount ΔE could lead to unbounded increases of variance and work fluctuations.

We point out that this is only the case if the system that we consider is infinite-dimensional. In the case of a finite d-dimensions system the worst increase of $\Delta\sigma$ at temperature $T = 0$ would be obtained for the superposition $|\psi\rangle = p\,|0\rangle + (1-p)\,|d-1\rangle$ resulting in

$$\left(\frac{\Delta\sigma_{\text{worst,d}}}{\omega}\right)^2 = \Big((d-1) - \Delta\epsilon\Big)\Delta\epsilon. \tag{4.55}$$

While the worst cases differ depending on whether the system's Hilbert space has finite or infinite dimension the best case coincides in both scenarios. The lowest increase in variance V resulting from a charging process is obtained by rotating to the superposition $|\psi\rangle = \sqrt{p}\,|n\rangle + \sqrt{(1-p)}\,|n+1\rangle$. The corresponding energy levels n, $(n+1)$ are just below, (above) the desired energy such that $n \leq E(\rho_f)\omega^{-1} \leq n+1$ with the probability

$$p = \lceil\Delta\epsilon\rceil - \Delta\epsilon \tag{4.56}$$

now fixed, and where $\lceil\Delta\epsilon\rceil$, ($\lfloor\Delta\epsilon\rfloor$) denotes to the ceiling (floor) function. The corresponding charging precision is then

$$\left(\frac{\Delta\sigma_{\text{best}}}{\omega}\right)^2 = (\Delta\epsilon - \lfloor\Delta\epsilon\rfloor)(\lceil\Delta\epsilon\rceil - \Delta\epsilon), \tag{4.57}$$

where we can see that by charging the battery by integer multiples m of ω such that $\Delta E = m\cdot\omega$ there is **no** change in charging precision i.e. $\Delta\sigma_{\text{best}} = 0$. The worst increase in variance when rotating to the superposition $|\psi\rangle = \sqrt{p}\,|n\rangle + \sqrt{(1-p)}\,|n+1\rangle$ is then obtained through charging the battery by $\Delta E = m\cdot\frac{\omega}{2}$. For more information on this topic see [1].

4.4.2 Precision Limits at Non-Zero Temperature

Now after having discussed the simplest case, let us consider an infinite-dimensional system at non-zero temperature. In this case equation (4.53) no longer holds, so we have to decide whether we consider a protocol that minimizes the charging precision **or** the work fluctuations during the charging process. In this section we will do the former while considering the case of thermal battery states now. One main difference when compared to the $T = 0$ (in units of ω) case is that our initial thermal state $\tau(\beta)$, which is diagonal in the energy eigenbasis, is now a mixed state.

It is trivial that the line of arguments made in the previous section about the worst case scenario for infinite-dimensions still holds true here. Charging the battery just by a little bit can lead to arbitrarily large increases in charging precision. In contrast even though the variance is upper bounded for finite-dimensional systems, the specifics are case-to-case dependent and as such can't be expressed in one closed expression like (4.55).

When it comes to the best case scenario things become more complicated. Generally speaking the goal is to find a state which minimizes the average, squared deviation [4] from the target energy and is in the unitary orbit of the initial thermal state for a fixed temperature T and input energy ΔE. Since there is no analytic solution to this problem, a protocol was proposed by Friis and Huber in [1], which allows one to obtain a minimal deviation state for fixed temperature and input energy which we shall discuss now.

Recall that our initial density operator $\tau(\beta) = \text{diag}\{P_0, P_1, P_2, ...\}$ is diagonal in the energy eigenbasis and it's entries are decreasing with increasing energy. Additionally, because the system's initial energy is determined by the temperature T we know that the desired final states energy is going to be $E(\tau(\beta)) + \Delta E = E(\rho_f)$. We then proceed to make two-level rotations on the (diagonal) entries of $\tau(\beta)$ in such a way that the largest P_0 gets shifted to the eigenstate that is closest to $E(\rho_f)$, the second largest P_1 gets shifted to the second closest eigenstate and so on. Unfortunately, even though ρ_f is a state in the unitary orbit of the initial thermal state that minimizes the deviation from the target energy as we wanted, its corresponding energy $E(\rho_f)$ is usually not the final energy we desire.

For the sake of clarity we will call the state with the unsatisfactory energy we have just obtained $\tilde{\rho_f}$ and the desired state ρ_f. Naturally, if the energy is not (yet) the correct one, then the minimal deviation from the target energy is not aswell. We point out that after this first part of the protocol, both cases $E(\tilde{\rho_f}) < E(\rho_f)$ and $E(\tilde{\rho_f}) > E(\rho_f)$ can occur. Therefore, in order to adjust the energy accordingly we need to apply a second sequence of two-level rotations which will increase the

[4] From now on whenever we use the term 'deviation' we will be referring to the average square deviation defined in (4.69).

deviation from the target energy. But since our goal is a state that minimizes the deviation from the target energy, the sequence starts with the rotations that have the most optimal value for $\frac{\Delta V}{\Delta E}$ and only if the desired energy still has not been reached this value changes. In other words, the first rotations that we make are the ones that yield the biggest shifts in energy ΔE (which can be positive or negative depending on the situation) while minimizing the increase in deviation from the target energy $\Delta \tilde{V}$. We keep doing this until the desired final energy has been reached.

The conclusion reached by Friis and M. Huber in [1] was that while in the best case scenario for $T = 0$ one can expect to find no change in charging precision for specific ΔE, the protocol proposed for the $T > 0$ case is able to **decrease** the charging precision to some degree with increasing temperature.

4.5 Minimal Precision Protocol for Finite Hilbert Spaces

In this section, we will present a protocol that extends the protocol given in [1] to the finite-dimensional case, that is, to d-dimensional systems with equally spaced energies.

The goal of this protocol is to raise the average energy of a single battery initially in the thermal state, while minimizing the variance of the final state.

As we have defined in 4.52, $\tau(\beta)$ is a density matrix corresponding to a thermal state, which is passive and thus diagonal in the Hamiltonian's energy eigenbasis with decreasing weights

$$P_n = \frac{1 - e^{-\beta\omega}}{1 - e^{-d\omega\beta}} \, e^{-n\beta\omega} \text{ for } n = 0, ..., d-1 \tag{4.58}$$

which lead to the initial temperature and dimension dependent energy

$$E(\tau(\beta)) = \frac{\omega}{e^{\omega\beta} - 1} - \frac{\omega d}{e^{d\beta\omega} - 1} \tag{4.59}$$

and initial energy variance

$$V(\tau(\beta)) = \frac{(e^{\omega\beta} - d^2 e^{d\omega\beta} + 2(-1 + d^2)e^{(1+d)\omega\beta} - d^2 e^{(2+d)\omega\beta} + e^{(\omega+2d\omega)\beta})\omega^2}{(e^{\omega\beta} - 1)^2 (e^{d\omega\beta} - 1)^2}, \tag{4.60}$$

where d denotes the dimension of the corresponding quantum battery.

We aim to find a state ρ_f with the desired energy

$$E(\rho_f) = E(\tau(\beta)) + \Delta E \tag{4.61}$$

by increasing the initial average energy by $\Delta E = \omega\Delta\epsilon$ through unitary operations, where $\rho_f = U\tau(\beta)U^\dagger$ and where ρ_f has the lowest variance of all states with the same average energy.

The protocol consists of two parts (part I and part II). Both parts consist of specific sequences of unitary two-level rotations between pairs of energy levels that either shift or completely re-order the respective weights P_n. Using unitary two-level rotations guarantees that any state reached at the end is in the unitary orbit of the initial state $\tau(\beta)$. As we shall see, in part I of the protocol entire weights will be re-ordered to new energy levels in such a way that the biggest weight P_0 ends up at the energy level which is closest to the desired energy $E(\rho_f) = \omega\,\epsilon$, the biggest after that P_1 will end up at the second closest energy level and so on.

Even though part I which re-orders entire pairs of weights at a time, is minimizing the deviation from the target energy, it is too imprecise to reach any desired energy. In fact in most cases the final energy following the sequence of part I $E(\tilde{\rho}_f) = \omega\,\tilde{\epsilon}$ will be either above or below the desired energy.

That is why we additionally need part II where the goal is to use another sequence of two-level rotations to fine-tune the current energy $\tilde{\epsilon}$ to the desired energy ϵ while still making sure we are minimizing the deviation from the target energy at each two-level rotation.

4.5.1 Protocol Part I

First we need to determine the energy level, which is closest to the desired energy ϵ, which we will call from now on k. Depending on the specific ϵ sometimes the closest energy level k will be below and sometimes above the desired energy, hence we define k as [1]

$$k = \begin{cases} \lfloor\epsilon\rfloor \text{ if } \epsilon - \lfloor\epsilon\rfloor < \lceil\epsilon\rceil - \epsilon \\ \lceil\epsilon\rceil \text{ if } \epsilon - \lfloor\epsilon\rfloor \geq \lceil\epsilon\rceil - \epsilon. \end{cases} \tag{4.62}$$

The value of k is of importance, because as previously mentioned, that is where the biggest weight P_0 will be assigned to.

The next step is to determine where on the ladder of energy levels k is. Here we stress the fact that the possible energy states of the finite, d-dimensional quantum battery we are considering form a ladder with equal energy gaps, which will play a significant role to us. Thus, if k fulfills condition

$$k \leq \frac{d-1}{2} \tag{4.63}$$

then k is in the 'lower half' of the ladder of energy levels, where the finite-dimensional nature of the battery will not impact the protocol significantly and we proceed with

part I proposed in [1] with the minor adjustment that the sum in the definition of the Hamiltonian (4.51) now ends at $d-1$.

As has been said, the goal of part I is to re-order weights P_n such that the biggest P_0 ends up at energy level k, which is closest to the desired energy ϵ, the next biggest P_1 is assigned to the next closest energy level and so on. Note that after the re-ordering is complete the density operator remains diagonal in the energy eigenbasis with new probability weights

$$\tilde{P}_n = \begin{cases} P_{2(k-n)-1} & \text{for} \quad n = 0, ..., k-1 \\ P_{2(n-k)} & \text{for} \quad n = k, ..., \max\{2k-1, d-1\} \\ P_n & \text{for} \quad n = 2k, ..., d-1 \end{cases} \tag{4.64}$$

for $k = \lceil \epsilon \rceil$, while in the case $k = \lfloor \epsilon \rfloor$ we have

$$\tilde{P}_n = \begin{cases} P_{2(k-n)} & \text{for} \quad n = 0, ..., k \\ P_{2(n-k)-1} & \text{for} \quad n = k+1, ..., \max\{2k, d-1\} \\ P_n & \text{for} \quad n = 2k+1, ..., d-1. \end{cases} \tag{4.65}$$

But should k violate condition (4.63), then k is in the 'upper half' of the ladder of energy levels, where we need to consider the boundary $n = d-1$ more carefully. Then, the probability weights after part I will take the form

$$\tilde{P}_n = \begin{cases} P_{d-n-1} & \text{for} \quad n = 0, ..., 2k-d-1 \\ P_{2(k-n)-1} & \text{for} \quad n = 2k-d, ..., k-1 \\ P_{2(n-k)} & \text{for} \quad n = k, ..., d-1 \end{cases} \tag{4.66}$$

for $k = \lceil \epsilon \rceil$, while in the case $k = \lfloor \epsilon \rfloor$ we obtain the distribution

$$\tilde{P}_n = \begin{cases} P_{d-n-1} & \text{for} \quad n = 0, ..., 2k-d \\ P_{2(k-n)} & \text{for} \quad n = 2k-d+1, ..., k \\ P_{2(n-k)-1} & \text{for} \quad n = k+1, ..., d-1. \end{cases} \tag{4.67}$$

The initial distribution of the thermal state is illustrated in Fig.4.4 while the resulting distribution after part I for $k > \frac{d-1}{2}$ and $k = \lceil \epsilon \rceil$ can be seen in Fig.4.5.

After part I has concluded we arrive at a new state $\tilde{\rho}$, which is in the unitary orbit of $\tau(\beta)$ and whose average energy is given by

$$\tilde{\epsilon} = \sum_n^{d-1} \tilde{P}_n n \tag{4.68}$$

and which minimizes the corresponding deviation from the target energy

$$\tilde{V} = \sum_n^{d-1} \tilde{P}_n (n-\epsilon)^2. \tag{4.69}$$

We define the change in charging precision as

$$\Delta\sigma = \sqrt{V(\rho_f)} - \sqrt{V(\tau(\beta))}, \tag{4.70}$$

however, as has been mentioned, $\tilde{\epsilon}$ rarely matches the desired energy ϵ hence a second part is necessary which fine-tunes the energy while minimizing the increase of deviation from the target energy.

4.5.2 Protocol Part II

As has been said before, the goal of part II is to adjust the average energy $\tilde{\epsilon}$ obtained in part I such that it reaches the desired value ϵ, through another sequence of two-level rotations. However, since the state reached in part I also minimized the deviation, we expect any additional energy shifts to increase this quantity. This is why the goal of the sequence proposed in part II is to minimize the increase in deviation from the target per unit energy change. Depending on whether we are in the $\tilde{\epsilon} < \epsilon$ or $\tilde{\epsilon} > \epsilon$ case after part I, the energy shift $\Delta\tilde{\epsilon}$ will be either positive or negative. Thus, in the former case we will minimize the quantity

$$\frac{\Delta\tilde{V}}{\Delta\tilde{\epsilon}} \tag{4.71}$$

while in the latter case we will maximize it.

Because the goal of the protocol in part II is to fine-tune the energy we will need to consider additionally smaller rotations between probability weights $\tilde{P}_n$,$\tilde{P}_m$ corresponding to energy levels n and m, which do not re-order them entirely but just shift certain amounts from one weight to the other. For this we consider

$$(\tilde{P}_n, \tilde{P}_m) \to (\cos^2\theta\tilde{P}_m + \sin^2\theta\tilde{P}_n, \cos^2\theta\tilde{P}_n + \sin^2\theta\tilde{P}_m), \tag{4.72}$$

which leads to the energy shift

$$\Delta\tilde{\epsilon} = \sin^2\theta(\tilde{P}_n - \tilde{P}_m)(m-n) \tag{4.73}$$

from which follows the corresponding increase of deviation from the target energy ϵ

$$\Delta\tilde{V} = \omega^2\sin^2\theta(\tilde{P}_n - \tilde{P}_m)((m-\epsilon)^2 - (n-\epsilon)^2). \tag{4.74}$$

With that in mind it is time that we parametrize the choice of energy levels to rotate between, that is, for fixed k we express the values

$$m = k - l, \tag{4.75}$$

$$n = k + l + j, \tag{4.76}$$

via two different values l and j according to (4.75)(4.76), where $j \in \mathbb{Z}$ and $l \in \mathbb{N}_0$. This parameterization can be done for any pair (m, n) but in the cases where $m < k$ and $n > k$, l corresponds to the minimum distance of one of them from k, and $j/2$ corresponds to the distance between k and the average of the values m and n.

Additionally, we demand that **always**

$$m < n. \tag{4.77}$$

Plugging the definitions of the energy levels (4.75) and (4.76) into (4.73) yields

$$\Delta\tilde{\epsilon} = \sin^2\theta(\tilde{P}_m - \tilde{P}_n)(2l + j), \tag{4.78}$$

where we know that $(2l + j) > 0$ because of condition (4.77). Straight forward algebra yields

$$\frac{1}{\omega^2}\frac{\Delta\tilde{V}}{\Delta\tilde{\epsilon}} = 2(k - \epsilon) + j, \tag{4.79}$$

which shows us that the value of interest depends on j but not on l. Since both cases $\tilde{\epsilon} < \epsilon$ and $\tilde{\epsilon} > \epsilon$ can occur we need to make a clear distinction here.

In the case of $\tilde{\epsilon} < \epsilon$ the energy needs to be increased, hence $\Delta\tilde{\epsilon} > 0$. From this follows that we can only consider two-level rotations in which $P_m > P_n$. Additionally, we need to choose j as small as possible in order to minimize $\frac{\Delta\tilde{V}}{\Delta\tilde{\epsilon}}$.

However, in the case of $\tilde{\epsilon} > \epsilon$ the energy has to be decreased, $\Delta\tilde{\epsilon} < 0$, from which follows that here only two-level rotations shall be considered for which $P_m < P_n$. But because this time $\Delta\tilde{\epsilon}$ is negative, we need to maximize j in order to obtain the most optimal value for (4.79).

For every two-level rotation the maximal possible energy shift $\Delta\tilde{\epsilon}_{\max}$ is calculated first. In case $\tilde{\epsilon} + \Delta\tilde{\epsilon}_{\max}$ exceeds the desired energy ϵ the rotation angle θ will be adjusted such that this is no longer the case. On the other hand if even the maximal amount is not enough, then a full swap $\theta = \frac{\pi}{2}$ takes place, and the protocol moves to the next rotation.

Inspection leads us to the following conclusion: the conditions we have discussed yield us for every case a different, initial pair of (j, l) that translates to the first pair of energy levels (m, n), which shall undergo a two-level rotation. Because (4.79) depends only on j, we will keep this value fixed, while changing l step by step by 1. Each new pair $(j, l \pm 1, 2, 3, ...)$ corresponds to a new pair of energy levels m and n. Only if the desired energy still has not been reached after the protocol has run out of energy levels, when either $m = 0$ or $n = d - 1$ has been reached j will be changed by 1 and the whole process starts over again.

From this it is clear that we are especially interested in determining the initial $(j, l_{\min})$ pair for each case and the final $(j, l_{\max})$ pair where the protocol runs out of

space and needs to change j by 1.

Going through the protocol case by case and keeping the condition (4.77) in mind we obtain that the first value for l is given by

$$l_{\min} = \begin{cases} 0 & \text{if} \quad k = \lfloor \epsilon \rfloor, \tilde{\epsilon} < \epsilon \\ 1 & \text{otherwise} \end{cases} \tag{4.80}$$

and does not depend on the condition whether k fulfills condition (4.63) or not.

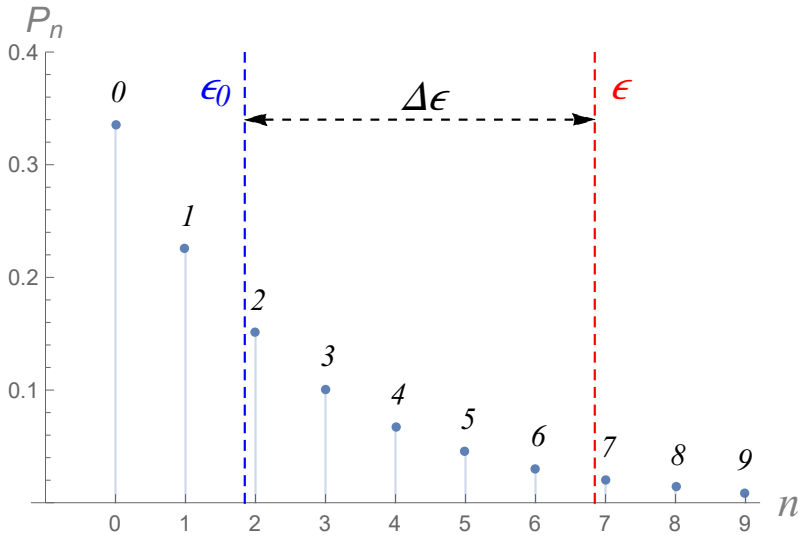


Figure 4.4: Intial thermal state: The initial thermal state $\tau(\beta)$ is given for a temperature $T = 2.5$ (in units of ω) and dimension $d = 10$. The probability weights P_n are decreasing with increasing energy, the blue dashed line marks the initial average energy ϵ_0 defined in (4.59). To illustrate the protocol we aim to increase the energy by $\Delta\epsilon$ to the desired energy ϵ marked by the red dashed line. Since one can see that the desired energy is closer to energy level 7 than to 6, we are in the case $k = \lceil \epsilon \rceil$.

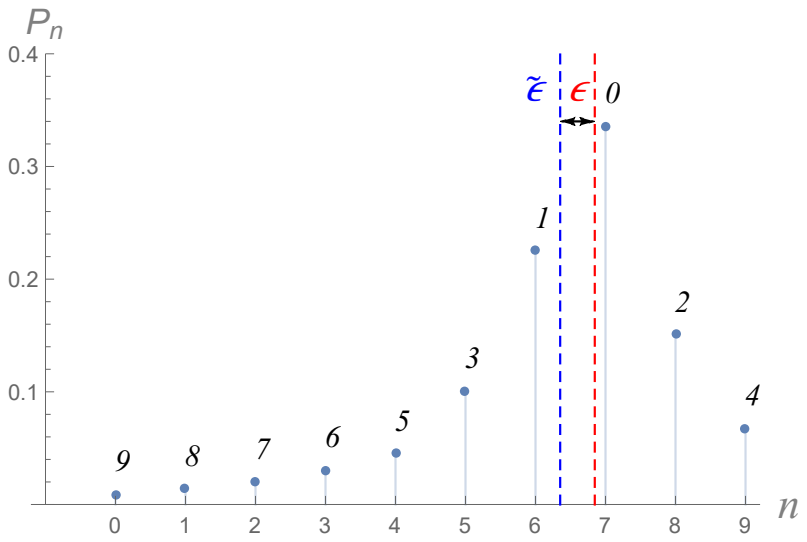


Figure 4.5: Distribution after part I: The first part of the protocol which re-orders entire probability weights at a time yields for the case defined in Fig.4.4 the following probability distribution. We note that the energy obtained here is lower than the desired energy, hence we are in the case $\tilde{\epsilon} < \epsilon$.

However, as has been mentioned, finding just one initial pair $(j, l_{\min})$ pair for which then l will be changed by 1 is sometimes not enough. Thus, we need to consider multiple 'phases' Φ of the protocol, where one phase corresponds to one fixed value of j such that

$$(j(\Phi), l_{min}(\Phi))) = \begin{cases} (\Phi, -\lceil \frac{\Phi}{2} \rceil + 1) & \text{if } \tilde{\epsilon} < \epsilon, k = \lfloor \epsilon \rfloor \\ (-\Phi + 1, \lceil \frac{\Phi}{2} \rceil) & \text{if } \tilde{\epsilon} > \epsilon, k = \lfloor \epsilon \rfloor \\ (\Phi - 1, -\lfloor \frac{\Phi}{2} \rfloor + 1) & \text{if } \tilde{\epsilon} < \epsilon, k = \lceil \epsilon \rceil \\ (-\Phi, \lfloor \frac{\Phi}{2} \rfloor + 1) & \text{if } \tilde{\epsilon} > \epsilon, k = \lceil \epsilon \rceil, \end{cases} \tag{4.81}$$

where the variable Φ denotes one 'phase' of rotations, for a fixed j. Once the protocol runs out of space (when either $m = 0$ or $n = d - 1$) Φ will be increased by one yielding a new initial pair $(j(2), l_{min}(2)))$ for which another round of rotations begins. The final distribution after part II of the protocol has concluded can be seen in Fig.4.6.

While the initial pair does not depend on the fact whether k obeys condition (4.63) this is no longer the case when determining l_{max}, which is responsible for reaching either end of the protocol.

If k is on the 'lower half' of the ladder of energy levels i.e. $k \leq \frac{d-1}{2}$, then energy level m will always reach 0 before n reaches $d - 1$ (or in the event of $k = \frac{d-1}{2}$, where m and n reach their respective boundaries simultaneously), which then yields

$$l_{max} = k \quad \text{for all cases.} \tag{4.82}$$

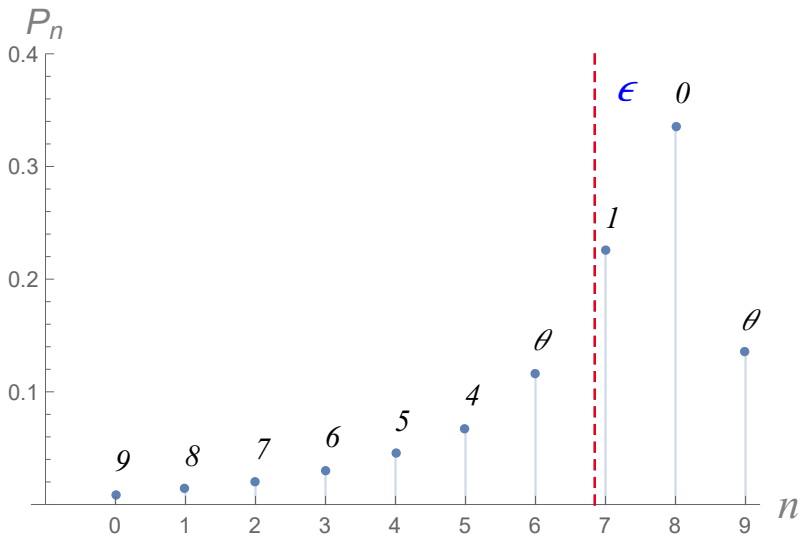


Figure 4.6: Final distribution after part II: Because the energy needs to be further increased part II of the protocol uses additional two-level rotations, which yield the desired result. For the first three rotations between energy levels $(m = 6, n = 8)$, $(m = 5, n = 9)$ and $(m = 7, n = 8)$ (where the third one already is part of phase two i.e. $\Phi = 2$) even the maximal rotation (complete re-arranging of entire weights) is not enough to reach the desired energy, hence the rotation angle for them is $\theta_l = \frac{\pi}{2}$. Finally, the fourth rotation $(m = 6, n = 9)$ is the final one for which the angle is $0 < \theta_l < \frac{\pi}{2}$ and shifts just parts of the weights from one level to the other.

But in the event of k being in the 'upper half' i.e. $k > \frac{d-1}{2}$ it will be n which reaches the limit of the energy ladder first. Since n depends on l and j here the case dependent solution is given by

$$l_{max} = \begin{cases} d-k-\Phi-1 & \text{if } \tilde{\epsilon} < \epsilon, k = \lfloor \epsilon \rfloor \\ d-k+\Phi-2 & \text{if } \tilde{\epsilon} > \epsilon, k = \lfloor \epsilon \rfloor \\ d-k-\Phi & \text{if } \tilde{\epsilon} < \epsilon, k = \lceil \epsilon \rceil \\ d-k+\Phi-1 & \text{if } \tilde{\epsilon} > \epsilon, k = \lceil \epsilon \rceil. \end{cases} \tag{4.83}$$

With all the tools at hand let us investigate the protocol of part II step by step:

1. Set $\Phi = 1$, calculate $(j(\Phi), l_{min}(\Phi)))$ and determine whether $k \leq \frac{d-1}{2}$.

2. If $\tilde{\epsilon} \neq \epsilon$ and as long $l \leq l_{max}$, where l_{max} is given by (4.82)(4.83), calculate the energy levels m and n, the maximal possible energy shift

$$\Delta\tilde{\epsilon}_{max} = (\tilde{P}_m - \tilde{P}_n)(2l + j) \tag{4.84}$$

and go to step 3.
In the case of $l > l_{max}$ while the desired energy still has not been reached, Φ is increased by one and the protocol goes back to step 1. If $\tilde{\epsilon} = \epsilon$ the protocol is finished and stops.

3. Here we need to yet again distinguish whether $\tilde{\epsilon} < \epsilon$ or $\tilde{\epsilon} > \epsilon$.

   In the case of $\tilde{\epsilon} < \epsilon$ the energy shift will be positive i.e. $\Delta\tilde{\epsilon} > 0$ and the angle θ_l is determined by

$$\theta_l = \begin{cases} \frac{\pi}{2} & \text{if} \quad \tilde{\epsilon} + \Delta\tilde{\epsilon}_{max} < \epsilon \\ \arcsin\sqrt{\frac{\epsilon - \tilde{\epsilon}}{\tilde{\epsilon}_{max}}} & \text{if} \quad \tilde{\epsilon} + \Delta\tilde{\epsilon}_{max} \geq \epsilon \end{cases} \tag{4.85}$$

   while in the case of $\tilde{\epsilon} > \epsilon$ the energy shift will be negative thus angle θ_l is given by

$$\theta_l = \begin{cases} \frac{\pi}{2} & \text{if} \quad \tilde{\epsilon} + \Delta\tilde{\epsilon}_{max} > \epsilon \\ \arcsin\sqrt{\frac{\epsilon - \tilde{\epsilon}}{\tilde{\epsilon}_{max}}} & \text{if} \quad \tilde{\epsilon} + \Delta\tilde{\epsilon}_{max} \leq \epsilon. \end{cases} \tag{4.86}$$

   After the appropriate angle has been calculated proceed with step 4.

4. Performing a two-level rotation between energy levels m and n with angle θ_l leads to the following changes:

$$\begin{aligned} \tilde{P_m} &\to \cos^2\theta\tilde{P}_m + \sin^2\theta\tilde{P}_n, \\ \tilde{P_m} &\to \cos^2\theta\tilde{P}_n + \sin^2\theta\tilde{P}_m, \\ \tilde{\epsilon} &\to \tilde{\epsilon} + \sin^2\theta_l + \tilde{\epsilon}_{max} = \Delta\tilde{\epsilon}^{\mathrm{I}}, \\ \tilde{V} &\to \tilde{V} + \Delta\tilde{\epsilon}^{\mathrm{I}}(2(k-\epsilon)+j). \end{aligned} \tag{4.87}$$

5. After all changes have been performed increase l by one and start over from step 2.

The protocol concludes when the desired energy has been reached or it has run out of allowed two-level rotations.

4.5.3 Results and Discussion

After we have studied the protocol in detail let us quickly summarize it. As previously discussed, the goal of the protocol is to charge a battery system in the initial state $\tau(\beta)$ by $\Delta\epsilon$ such that the final state ρ_f with the desired energy $\epsilon_0 + \Delta\epsilon = \epsilon$, where $E(\tau(\beta)) = \omega\epsilon_0$, minimizes the deviation and is in the unitary orbit of the initial state. To this end we use a protocol in which we distinguish between two parts:

Part I: The goal of the first part of the protocol is to assign the probability weights P_n around the desired energy ϵ such that the biggest weight P_0 is shifted to the eigenstate closest to ϵ, the next biggest P_1 gets shifted to the next closest eigenstate

and so on. Here, we stress the fact that during this process the sizes of the weights remain unchanged. Additionally, it is worth pointing out that the rotations used in this part of the protocol are, in principle, able to decrease the deviation from the target energy such that the deviation of the final state $V(\rho_f)$ is as low or even lower than the deviation of the initial state $V(\tau(\beta))$.

Part II: Because the first part is generally not enough to reach the exact desired energy we distinguish between the cases $\tilde{\epsilon} < \epsilon$ and $\tilde{\epsilon} > \epsilon$, where $\tilde{\epsilon}$ is the energy after part I. In either case part II rotates between two energy levels at a time (4.75)(4.76) such that again the entire probability weights get exchanged, *except* for the last rotation for which the system's energy would surpass the desired energy if the entire weights were shifted. Instead an appropriate rotation angle θ is determined (4.85)(4.86) by which the two weights get rotated.

Now with the necessary knowledge at hand let us discuss the behavior of the deviation of the final state ρ_f by charging batteries for values $\Delta\epsilon = \{0.01, ..., \Delta\epsilon_{\max}\}$, where $\Delta\epsilon_{\max}$ denotes the maximal value with which the corresponding battery can be charged. We will define $\Delta\epsilon_{\max}$ in (4.89).

First, we shall investigate the deviation at different temperatures for fixed dimensions $d = 10$ displayed in Fig.4.7. As has been already shown in section 4.4.2, the thermal state $\tau(\beta)$ takes the form of a pure state for $T = 0$, is mixed for $T > 0$ and approaches the maximally mixed state for $T \to \infty$. This property is of importance to us because of multiple reasons. First, since pure states have vanishing variance, one can expect that by charging the battery by integer multiples of the oscillator frequency, such that the final state corresponds to an eigenstate the change in standard deviation will be $\Delta\sigma = 0$. Second, because the batteries we are considering now have a finite-dimensional Hilbert spaces they cannot be charged by any arbitrarily large amount, which means that additionally to the initial energy given by (4.59) one needs to consider the maximal possible, temperature and dimension-dependent energy which is given by

$$[E(\rho_f)]_{\max} = \frac{e^{\beta\omega}(1 - d\, e^{(-1+d)\omega\beta} + (-1+d)e^{d\omega\beta})\omega}{(e^{\omega\beta} - 1)(e^{d\omega\beta} - 1)}. \tag{4.88}$$

Because pure states are the only states that can occupy only one energy state at a time they minimize the initial energy and maximize the possible final energy. In other words, the maximal amount of energy a given battery can be charged with

$$[E(\rho_f)]_{\max} - E(\tau(\beta)) = \Delta E_{\max}, \tag{4.89}$$

where $\Delta E_{\max} = \omega\Delta\epsilon_{\max}$ is maximized for pure states.

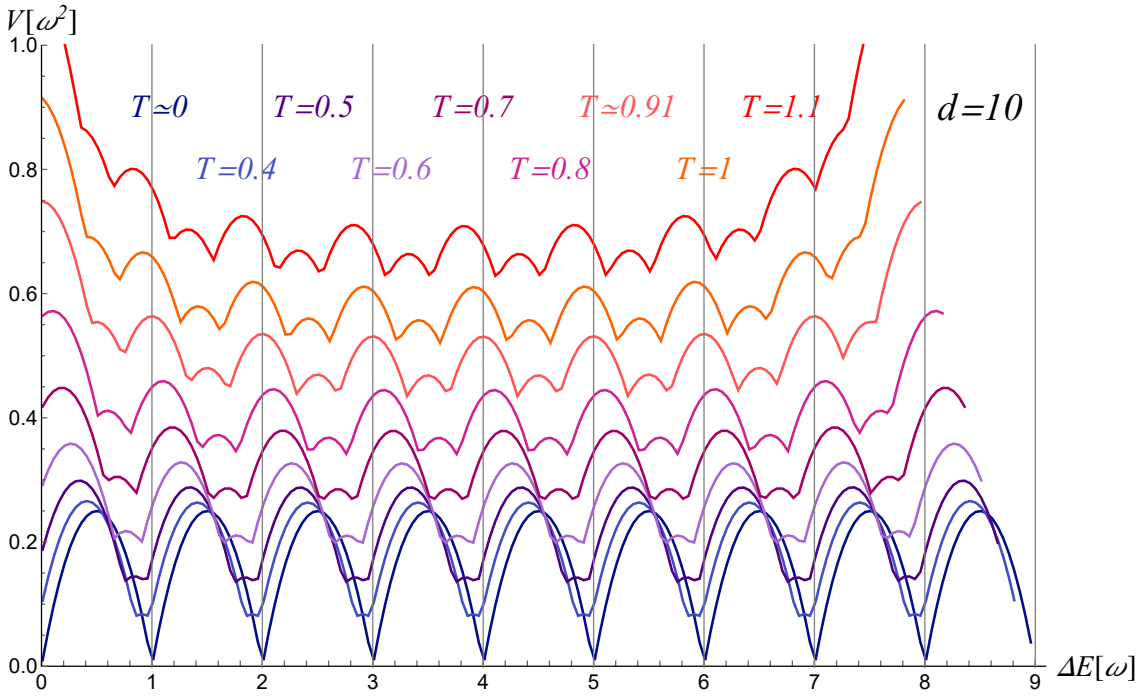
Additionally, the further we increase the temperature, the more mixed the initial state becomes. With this also the initial energy increases, while the maximal energy decreases i.e. the higher the temperature the lower $\Delta\epsilon_{\max}$.

Now let us discuss the general behavior of the deviation for higher temperatures in Fig.4.7. As has been mentioned, the rotations used in part I are able to decrease the deviation such that, under certain conditions, which we shall now investigate, the final state's deviation can be lower than the initial state's deviation.

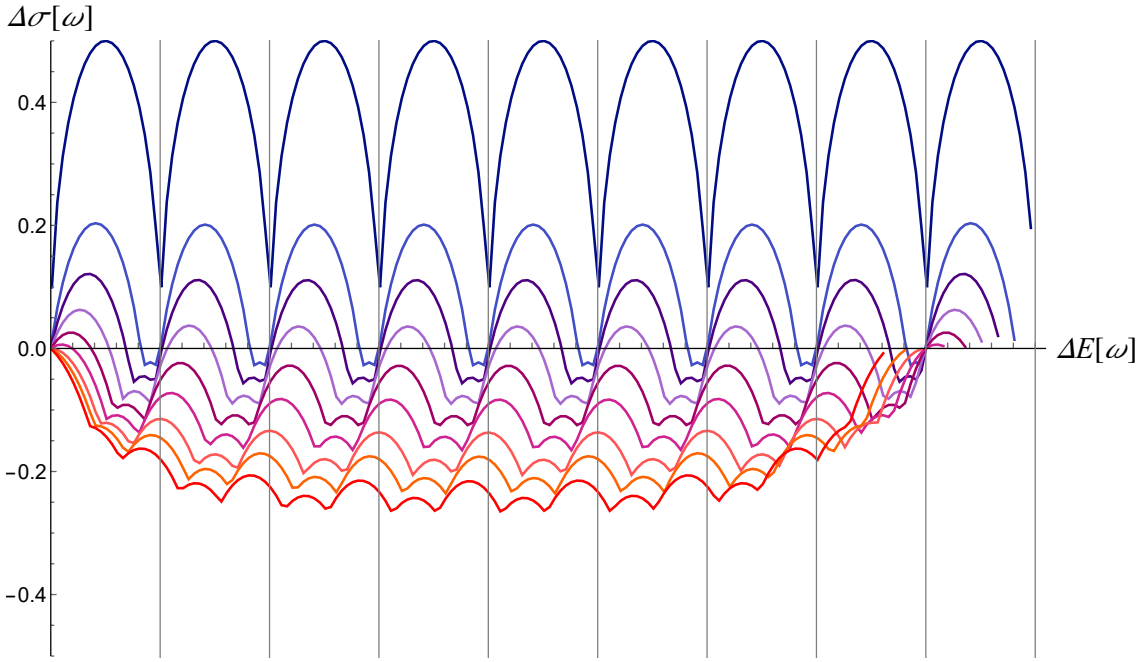
In order to be able to observe this effect, the first condition is that the temperature and with that the initial deviation must be non-zero. As we have discussed in section 4.4.1 only for $T = 0$ the initial deviation represents also a minimum.

The second condition is that the desired final state ϵ must be 'far enough' from either end of the ladder of energy levels. As can be seen in Fig.4.7 for higher temperatures, the deviation first decreases but increases towards the end again, where 'end' denotes the maximal possible amount $\Delta\epsilon_{\max}$ a battery can be charged with. Unsurprisingly $\Delta\epsilon_{\max}$ decreases as the temperature increases. 'Far enough from either boundary of the ladder of energy levels' roughly speaking means that the protocol in part I must have enough space to *sensibly* rotate as many finite probability weights as possible. Sensibly here means that the two-level rotations of part I can be divided into two groups: 1. The actual deviation minimizing rotations, which alternate between placing the weights to energy levels that are above/below the target energy ϵ and 2. The 'left-over' rotations where the protocol ran out of space. In Fig.4.5 deviation minimizing rotations placed the weights to the energy levels $n = 4, 5, .., 9$ while the remaining weights were placed to energy levels $n = 0, .., 3$ by the' left-over' rotations.

This becomes very clear when considering a case in which a battery gets charged with the maximal amount $\Delta\epsilon_{\max}$. Even though **every** weight got re-assigned to a new place by the protocol in part I, each of these rotations was a 'left-over' rotation which is not able to lower the deviation. For dimensions $d = 10$ shown in 4.7 this effectively means that one can expect the best results in terms of deviation from ϵ for values $\Delta\epsilon$ which place the desired final energy ϵ in the 'middle' of the ladder of energy levels, which equals to charging the battery by half of it's maximal capacity $\frac{\Delta\epsilon_{\max}}{2}$. There the protocol of part I has the most space for *sensible* rotations. This observation then holds true for any d and non-zero T.
We stress here the fact that our analysis describes a trend and is not an exact statement. The specifics of each process need to be worked out on a case-by-case basis.



(a) Optimal variance achievable for different temperatures at fixed d.



(b) Optimal change in precision achievable for different temperatures at fixed d.

Figure 4.7: **Optimal charging precision for different temperatures, at $d = 10$.** In (a) the minimal obtainable variance V (in units of ω^2) and in (b) the standard deviation change $\Delta\sigma$ (in units of ω) defined in (4.70) are plotted for different temperatures. V and $\Delta\sigma$ are plotted against the energy input $\Delta E/\omega$. The exact numerical value of temperature $T \approx 0$ is $T = 0.001$ (in units of ω) and of temperature $T \approx 0.91$ is $T = 0.910427$ (in units of ω).

Additionally, notice that in Fig.4.7 the temperature $T \approx 0.91$ (in units of ω) is not precisely given. This is based on the fact that this temperature poses a boundary such that for dimension $d = 10$ the curve for the minimal variance in 4.7 (a) is always below the initial variance for temperatures $T \approx 0.91$ or higher.

Temperature $T \approx 0.91$ (in units of ω) has been obtained by solving for which T the initial energy given by (4.59) fulfills $E(\tau(\beta)) = 0.5$ (in units of ω), for $d = 10$. This has been done because for this temperature (and any temperature above), for small $\Delta\epsilon = 0.01$, k becomes non-zero. In other words for any temperature below $T \approx 0.91$ for small $\Delta\epsilon$, we obtain $k = 0$ for which part I performs *no* rotations which could lower the variance. However, for non-zero k, for small $\Delta\epsilon$, part I is able to perform rotations and thus a decrease in variance is possible from the very beginning of the plot in Fig.4.7.

In the same fashion the respective 'boundary' temperatures for other dimension, have been calculated and plotted in Fig.4.8.

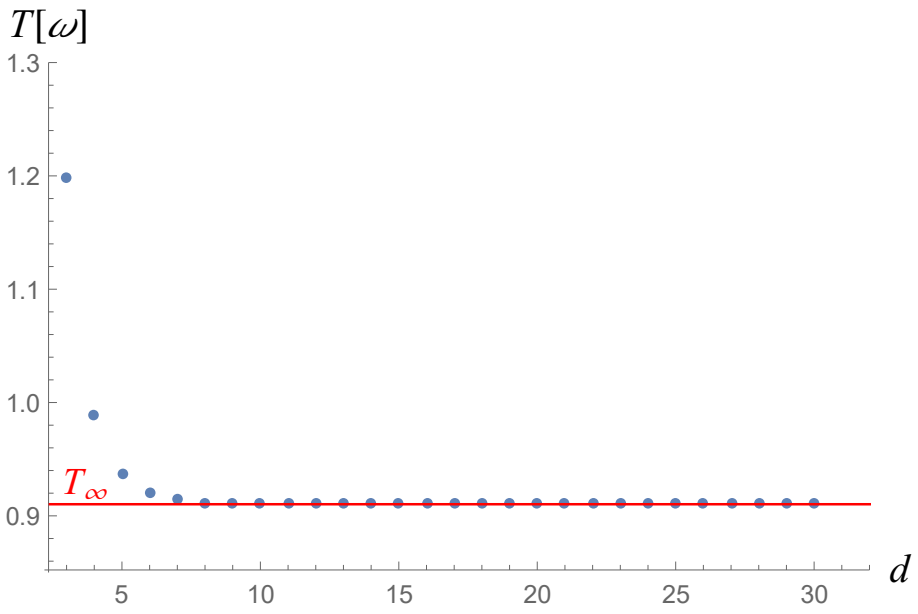
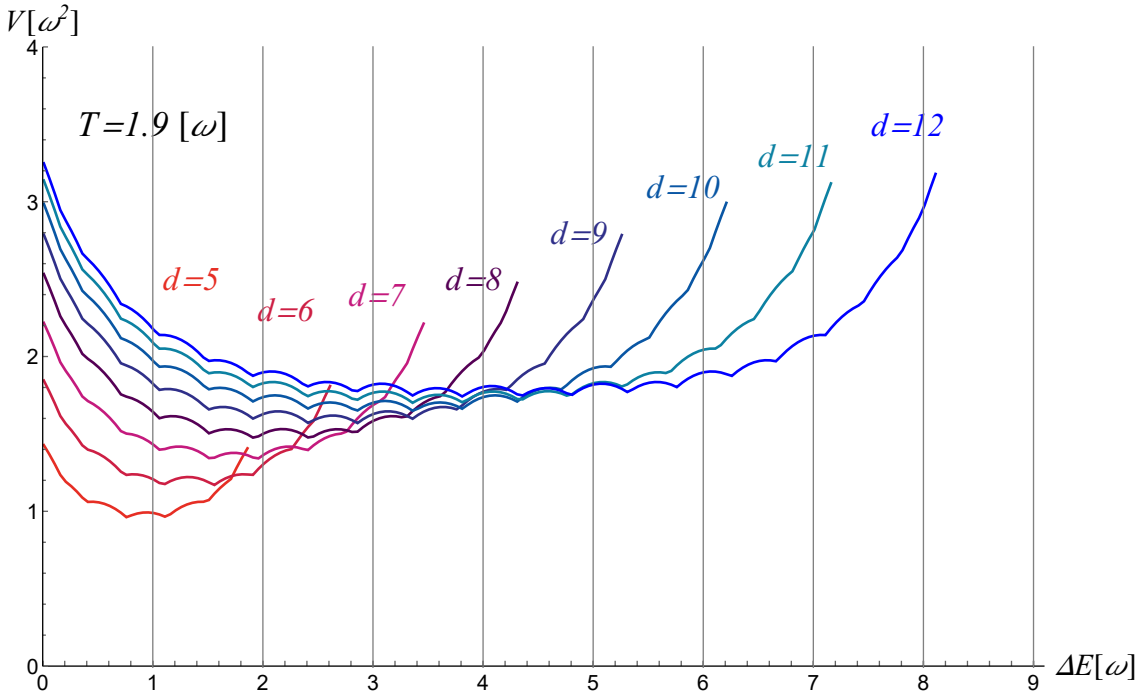
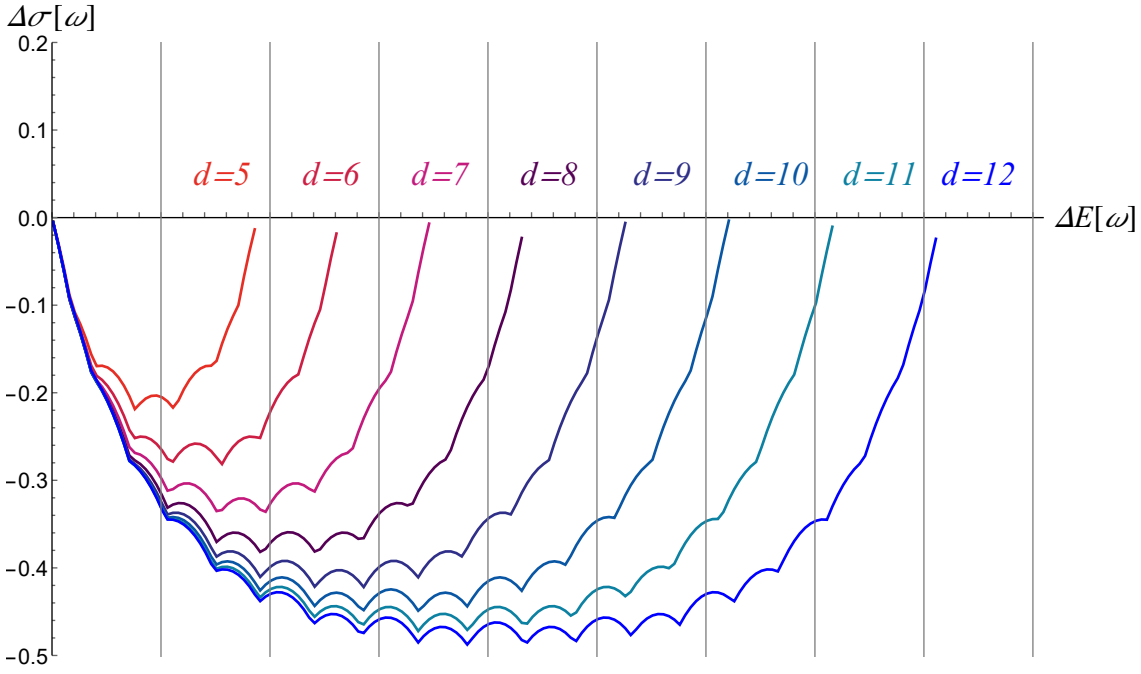


Figure 4.8: **'Boundary' temperature for different dimensions**. Temperatures (in units of ω) obtained by solving $E(\tau(\beta)) = 0.5$ (in units of ω) given in (4.59) for different dimensions d, are plotted against $d = \{3, 4, ..., 30\}$. The 'boundary' temperature denotes a temperature for which the curve for the minimal variance in 4.7 (a) is always below the initial variance. This is then also true for any temperature above the 'boundary' temperature, for the same d. The red line labeled as T_∞ denotes the the 'boundary' temperature in the limit $d \to \infty$ and has the value $T = 0.9102392$ (in units of ω).

Now we shall investigate the variance at different dimension for a fixed temperature $T = 1.9$ (in units of ω) displayed in Fig.4.9. In agreement with our previous discussion the variance decreases for values of $\Delta\epsilon$, which place the final energy in the 'middle' of the respective ladders of energy levels. The initial variances represent maxima when we are past the temperatures plotted in 4.8 for the corresponding dimension d, which act as boundaries between the cases where part I is not able to do any sensible rotations and the cases where it is for small $\Delta\epsilon$.



(a) Optimal variance achievable for different dimensions at fixed T.



(b) Optimal change in precision achievable for different dimensions at fixed T.

Figure 4.9: **Optimal charging precision for different dimensions at temperature $T = 1.9$** (in units of ω). In (a) the minimal variance V (in units of ω^2) and in (b) the standard deviation change $\Delta\sigma$ (in units of ω) defined in (4.70) are plotted against the energy input $\Delta E/\omega$, for different dimensions d.

Chapter 5

Conclusion

Quantum thermodynamics is a field which attempts to understand the connection between the microscopic description provided by quantum mechanics and the macroscopic laws of thermodynamics [6][9][10]. At its core lies the topic of energy extraction from [4][68] and energy charging into [18][67] quantum mechanical systems, we call *quantum batteries*. While studying these tasks, we discussed the concept of passive states [28], states from which no more energy can be extracted. Additionally, because tensor products of passive states are not necessarily passive, an extension called complete passivity [27][6] was discussed in this thesis.

The central goal of this thesis was to was to develop a unitary battery charging protocol that raises the average energy of a finite-dimensional quantum battery initially in a completely passive state, while additionally minimizing the energy variance of the final state. To this end we have developed a protocol based on [1], which uses sequences of (non-unique) unitary, two-level rotations to reach the desired final state.

The results obtained by this optimal protocol for the finite-dimensional case are presented in section 4.5.3 for selected exemplary dimensions/temperatures. A curve for the minimal variance of the final state, and the optimal standard deviation change are plotted against the energy input for different dimension and temperatures in 4.7 and 4.9. Our investigation has shown that the protocol can lead to a decrease of variance when compared to the initial state for non-zero temperatures. Generally speaking a trend of decreasing variances can be observed for any input energy up until the battery has been charged to half of its maximal capacity. In contrast to the infinite-dimensional case in [1], where the battery has no maximal capacity, charging the battery past this amount will result in a trend of increasing variances.

We point out that these optimal protocols generally have a complicated form which depends on the specific dimension, temperature and desired target energy of the battery, and may be difficult to realize in practical laboratory settings. However, the protocols are of fundamental interest because they provide an insight about

charging precisions that are obtainable in principle. Thus, the results presented in this thesis provide a benchmark for realizable protocols, which would be measured against these optimal protocols in a laboratory setting.

Finally we hope that our results might motivate further research into this topic such as considering charging multiple, finite-dimensional batteries at once or allow for Hamiltonians with degenerate energy levels.

Bibliography

[1] Nicolai Friis and Marcus Huber. Precision and Work Fluctuations in Gaussian Battery Charging. *Quantum*, 2:61, April 2018. arXiv: 1708.00749.

[2] A.F.J. Levi. *Applied Quantum Mechanics*. Cambridge University Press, 2003, 2003, Page xiii.

[3] Robert Alicki and Ronnie Kosloff. Introduction to Quantum Thermodynamics: History and Prospects. *arXiv:1801.08314 [quant-ph]*, January 2018. arXiv: 1801.08314.

[4] Robert Alicki and Mark Fannes. Extractable work from ensembles of quantum batteries. Entanglement helps. *Physical Review E*, 87(4), April 2013. arXiv: 1211.1209.

[5] Bartłomiej Gardas and Sebastian Deffner. Thermodynamic universality of quantum Carnot engines. *Physical Review E*, 92(4), October 2015. arXiv: 1503.03455.

[6] John Goold, Marcus Huber, Arnau Riera, Lídia del Rio, and Paul Skrzypczyk. The role of quantum information in thermodynamics — a topical review. *Journal of Physics A: Mathematical and Theoretical*, 49(14):143001, April 2016. arXiv: 1505.07835.

[7] A. E. Allahverdyan. Nonequilibrium quantum fluctuations of work. *Phys. Rev. E*, 90:032137, Sep 2014.

[8] Michele Campisi, Peter Hänggi, and Peter Talkner. Colloquium. Quantum Fluctuation Relations: Foundations and Applications. *Reviews of Modern Physics*, 83(3):771–791, July 2011. arXiv: 1012.2268.

[9] Peter Talkner, Eric Lutz, and Peter Hanggi. Fluctuation theorems: Work is not an observable. *Physical Review E*, 75(5), May 2007. arXiv: cond-mat/0703189.

[10] C. Gogolin and J. Eisert. Equilibration, thermalisation, and the emergence of statistical mechanics in closed quantum systems. *Reports on Progress in Physics*, 79(5):056001, May 2016. arXiv: 1503.07538.

[11] D. Tong. Statistical Physics, University of Cambridge Part II Mathematical Tripos. `http://www.damtp.cam.ac.uk/user/tong/statphys/one.pdf`. Last accessed: 2019-01-30.

[12] Noah Linden, Sandu Popescu, Anthony J. Short, and Andreas Winter. Quantum mechanical evolution towards thermal equilibrium. *Physical Review E*, 79(6), June 2009. arXiv: 0812.2385.

[13] Nelly Ng and Mischa P. Woods. Resource theory of quantum thermodynamics: Thermal operations and Second Laws. *arXiv:1805.09564 [quant-ph]*, May 2018. arXiv: 1805.09564.

[14] Giuseppe Vitagliano, Claude Klöckl, Marcus Huber, and Nicolai Friis. Trade-off Between Work and Correlations in Quantum Thermodynamics. *arXiv:1803.06884 [quant-ph]*, March 2018. arXiv: 1803.06884.

[15] Karen V. Hovhannisyan, Martí Perarnau-Llobet, Marcus Huber, and Antonio Acín. Entanglement Generation is Not Necessary for Optimal Work Extraction. *Physical Review Letters*, 111(24), December 2013. arXiv: 1303.4686.

[16] Paul Skrzypczyk, Anthony J. Short, and Sandu Popescu. Extracting work from quantum systems. *arXiv:1302.2811 [quant-ph]*, February 2013. arXiv: 1302.2811.

[17] Paul Skrzypczyk, Anthony J. Short, and Sandu Popescu. Work extraction and thermodynamics for individual quantum systems. *Nature Communications*, 5:4185, June 2014.

[18] Felix C Binder, Sai Vinjanampathy, Kavan Modi, and John Goold. Quantacell: powerful charging of quantum batteries. *New Journal of Physics*, 17(7):075015, July 2015.

[19] Robert Alicki and Mark Fannes. Entanglement boost for extractable work from ensembles of quantum batteries. *Phys. Rev. E*, 87:042123, Apr 2013.

[20] Matteo Lostaglio. Quantum fluctuation theorems, contextuality and work quasi-probabilities. *Physical Review Letters*, 120(4), January 2018. arXiv: 1705.05397.

[21] G N Bochkov and E Kuzovlev. General theory of thermal fluctuations in nonlinear systems. 45(1):6, 1977.

[22] Martí Perarnau-Llobet, Elisa Bäumer, Karen V. Hovhannisyan, Marcus Huber, and Antonio Acin. No-go theorem for the characterization of work fluctuations in coherent quantum systems. *Phys. Rev. Lett.*, 118:070601, Feb 2017.

[23] L. D. Landau and E. M. Lifshitz. *Statistical Physics*. 01 1980.

[24] David J. Griffiths. *Introduction to Quantum Mechanics (2nd Edition)*. Pearson Prentice Hall, 2nd edition, April 2004.

[25] R Alicki. The quantum open system as a model of the heat engine. *Journal of Physics A: Mathematical and General*, 12(5):L103–L107, May 1979.

[26] H. Goldstein, C.P. Poole, and J.L. Safko. *Klassische Mechanik*. Wiley, 2012.

[27] Paul Skrzypczyk, Ralph Silva, and Nicolas Brunner. A short note on passivity, complete passivity and virtual temperatures. *Physical Review E*, 91(5), May 2015. arXiv: 1412.5485.

[28] W. Pusz and Woronowicz. Passive states and KMS states for general quantum systems. *Commun. Math. Phys.*, 58:273, 1977.

[29] A. Lenard. Thermodynamical proof of the gibbs formula for elementary quantum systems. *Stat. Phys.*, 19:575, 1978.

[30] N. Friis A. Bertlmann. Theoretical Physics T2, Quantum Mechanics, University of Vienna. `https://homepage.univie.ac.at/reinhold.bertlmann/pdfs/T2_Skript_Ch_9corr.pdf`. Last accessed: 2019-01-30.

[31] A. Einstein, B. Podolsky, and N. Rosen. Can quantum-mechanical description of physical reality be considered complete? *Phys. Rev.*, 47:777–780, May 1935.

[32] J.S. Bell. On the Einstein Podolsky Rosen Paradox. *Physics Publishing Co.*, 1:6, Nov 1964. `https://cds.cern.ch/record/111654/files/vol1p195-200_001.pdf`. Last accessed: 2019-01-30.

[33] Charles H. Bennett, David P. DiVincenzo, John A. Smolin, and William K. Wootters. Mixed State Entanglement and Quantum Error Correction. *Physical Review A*, 54(5):3824–3851, November 1996. arXiv: quant-ph/9604024.

[34] Nicolai Friis, Sridhar Bulusu, and Reinhold A. Bertlmann. Geometry of two-qubit states with negative conditional entropy. *Journal of Physics A Mathematical and Theoretical*, 50:125301, 02 2017.

[35] Ross Dorner and Vlatko Vedral. Correlations in Quantum Physics. *International Journal of Modern Physics B*, 27:1345017, January 2013. arXiv: 1208.4961.

[36] Kavan Modi, Hugo Cable, Mark Williamson, and Vlatko Vedral. Quantum Correlations in Mixed-State Metrology. *Physical Review X*, 1(2), December 2011.

[37] C. Jarzynski. A nonequilibrium equality for free energy differences. *Physical Review Letters*, 78(14):2690–2693, April 1997. arXiv: cond-mat/9610209.

[38] Gavin E. Crooks. The Entropy Production Fluctuation Theorem and the Nonequilibrium Work Relation for Free Energy Differences. *Physical Review E*, 60(3):2721–2726, September 1999. arXiv: cond-mat/9901352.

[39] Gavin E. Crooks. Entropy production fluctuation theorem and the nonequilibrium work relation for free energy differences. *Phys. Rev. E*, 60:2721–2726, Sep 1999.

[40] Sebastian Deffner. Nonequilibrium entropy production in open and closed quantum systems. `https://d-nb.info/101192949X/34`, Dez 2010. Last accessed: 2019-01-30.

[41] Denis J. Evans, E. G. D. Cohen, and G. P. Morriss. Probability of second law violations in shearing steady states. *Phys. Rev. Lett.*, 71:2401–2404, Oct 1993.

[42] Tameem Albash, Daniel A. Lidar, Milad Marvian, and Paolo Zanardi. Fluctuation theorems for quantum processes. *Phys. Rev. E*, 88:032146, Sep 2013.

[43] Christopher Jarzynski. Nonequilibrium work relations: Foundations and applications. *Eur. Phys. J. B*, 64:331–340, 08 2008.

[44] Satoshi Yukawa. A Quantum Analogue of the Jarzynski Equality. *Journal of the Physical Society of Japan*, 69(8):2367–2370, 2000.

[45] Peter Talkner and Peter Hanggi. The Tasaki-Crooks quantum fluctuation theorem. *arXiv:0705.1252 [cond-mat]*, May 2007. arXiv: 0705.1252.

[46] P. Solinas and S. Gasparinetti. Full distribution of work done on a quantum system for arbitrary initial states. *Phys. Rev. E*, 92:042150, Oct 2015.

[47] Álvaro M. Alhambra, Lluis Masanes, Jonathan Oppenheim, and Christopher Perry. Fluctuating work: From quantum thermodynamical identities to a second law equality. *Phys. Rev. X*, 6:041017, Oct 2016.

[48] Yelena Guryanova, Nicolai Friis, and Marcus Huber. Ideal Projective Measurements Have Infinite Resource Costs. *arXiv:1805.11899 [quant-ph]*, May 2018. arXiv: 1805.11899.

[49] Augusto J. Roncaglia, Federico Cerisola, and Juan Pablo Paz. Work measurement as a generalized quantum measurement. *Physical Review Letters*, 113(25), December 2014. arXiv: 1409.3812.

[50] Yakir Aharonov, David Z. Albert, and Lev Vaidman. How the result of a measurement of a component of the spin of a spin-1/2 particle can turn out to be 100. *Phys. Rev. Lett.*, 60:1351–1354, Apr 1988.

[51] Justin Dressel, Mehul Malik, Filippo M. Miatto, Andrew N. Jordan, and Robert W. Boyd. Colloquium: Understanding quantum weak values: Basics and applications. *Rev. Mod. Phys.*, 86:307–316, Mar 2014.

[52] Henry Margenau and Robert Nyden Hill. Correlation between measurements in quantum theory. *Progress of Theoretical Physics*, 26(5):722–738, 1961.

[53] Martí Perarnau-Llobet. Thermodynamics and Quantum Correlations, Polytechnic University of Catalonia. `https://upcommons.upc.edu/bitstream/handle/2117/107050/TMPL1de1.pdf?sequence=1&isAllowed=y`, Apr 2016. Last accessed: 2019-01-30.

[54] B Scrosati C.A. Vincent. *Modern Batteries: An Introduction to Electrochemical Power Sources*. John Wiley & Sons, Inc., 1997, page 351.

[55] W. Grimus. *Einführung in die Statistische Physik und Thermodynamik*. Oldenbourg, 2010.

[56] Martí Perarnau-Llobet, Karen V. Hovhannisyan, Marcus Huber, Paul Skrzypczyk, Jordi Tura, and Antonio Acín. Most energetic passive states. *Physical Review E*, 92(4), October 2015. arXiv: 1502.07311.

[57] Martí Perarnau-Llobet, Karen V. Hovhannisyan, Marcus Huber, Paul Skrzypczyk, Nicolas Brunner, and Antonio Acín. Extractable Work from Correlations. *Physical Review X*, 5(4), October 2015. arXiv: 1407.7765.

[58] Marcus Huber, Martí Perarnau-Llobet, Karen V. Hovhannisyan, Paul Skrzypczyk, Claude Klöckl, Nicolas Brunner, and Antonio Acín. Thermodynamic cost of creating correlations. *New Journal of Physics*, 17(6):065008, June 2015. arXiv: 1404.2169.

[59] Lieven Clarisse, Sibasish Ghosh, Simone Severini, and Anthony Sudbery. Entangling Power of Permutations. *Physical Review A*, 72(1), July 2005. arXiv: quant-ph/0502040.

[60] V. Vedral, M. B. Plenio, M. A. Rippin, and P. L. Knight. Quantifying Entanglement. *Physical Review Letters*, 78(12):2275–2279, March 1997. arXiv: quant-ph/9702027.

[61] V. Vedral, M. B. Plenio, K. Jacobs, and P. L. Knight. Statistical Inference, Distinguishability of Quantum States, And Quantum Entanglement. *Physical Review A*, 56(6):4452–4455, December 1997. arXiv: quant-ph/9703025.

[62] Steven M. Girvin. The Quantum Hall Effect: Novel Excitations and Broken Symmetries. *arXiv:cond-mat/9907002*, July 1999. arXiv: cond-mat/9907002.

[63] S. Kullback and R. A. Leibler. On information and sufficiency. *Ann. Math. Statist.*, 22(1):79–86, 03 1951.

[64] Tzu-Chieh Wei, Marie Ericsson, Paul M. Goldbart, and William J. Munro. Connections between relative entropy of entanglement and geometric measure of entanglement. *arXiv:quant-ph/0405002*, April 2004. arXiv: quant-ph/0405002.

[65] L. Mandelstam and Ig. Tamm. *The Uncertainty Relation Between Energy and Time in Non-relativistic Quantum Mechanics*, pages 115–123. Springer Berlin Heidelberg, 1991.

[66] Norman Margolus and Lev B. Levitin. The maximum speed of dynamical evolution. *Physica D: Nonlinear Phenomena*, 120(1-2):188–195, September 1998. arXiv: quant-ph/9710043.

[67] Francesco Campaioli, Felix A. Pollock, Felix C. Binder, Lucas C. Céleri, John Goold, Sai Vinjanampathy, and Kavan Modi. Enhancing the charging power of quantum batteries. *Physical Review Letters*, 118(15), April 2017. arXiv: 1612.04991 Citation Key: CampaioliEnhancingchargingpower2017.

[68] Paul Skrzypczyk, Anthony J. Short, and Sandu Popescu. Extracting work from quantum systems. *arXiv:1302.2811 [quant-ph]*, February 2013. arXiv: 1302.2811.