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***Analysis of a Measurement-based Quantum
Otto Cycle With a Single-bath***

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Rio de Janeiro - RJ
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RESUMO

No presente trabalho, nós iremos apresentar uma breve revisão de uma área recente na física - a termodinâmica quântica. Nosso estudo se inicia com os conceitos básicos da termodinâmica clássica, passando pelas definições de calor, trabalho e pressão no regime da mecânica quântica, importantes teoremas de flutuação, até uma importante aplicação da termodinâmica quântica, as máquinas térmicas quânticas. Após essa introdução, iremos apresentar um protocolo recém-proposto de uma máquina térmica baseada em medida que funciona com apenas um banho térmico. Em seguida, iremos utilizar um sistema quântico de três níveis aplicado à essa máquina baseada em medida, com o propósito de mostrar que é possível alcançar e ultrapassar a eficiência de uma máquina térmica que utiliza um sistema de dois níveis como substância de trabalho acoplado a dois banhos térmicos à temperaturas T_c e T_h . Além disso, mostramos que, mesmo utilizando o mesmo sistema de três níveis, a eficiência da máquina acoplada aos dois banhos pode ser ultrapassada pela máquina baseada em medida. Na verdade, qualquer sistema com mais de dois níveis pode apresentar uma melhoria na sua eficiência se considerarmos certas condições específicas. O resultado principal é mostrar que é possível explicar o aumento de eficiência sem precisar invocar argumentos baseados em emaranhamento ou outros efeitos provenientes da mecânica quântica, como coerência quântica e discórdia, como já foi assumido em trabalhos anteriores.

ABSTRACT

In the present work, we present a brief review of the new emerging field in physics - quantum thermodynamics. Our study starts from the basic concepts of classical thermodynamics, going through quantum thermodynamics definitions of work, heat and pressure, some important fluctuation theorems, and up to one important application of this field, quantum thermal machines. After this review, we present a recently proposed single-bath measurement-based quantum Otto engine without feedback control. Applying it to a three-level quantum system, we aim to show that, by this new measurement-based engine, it is possible to surpass the two-level Otto efficiency limit working between two thermal baths at temperatures T_c and T_h . We also show that the efficiency can be greater than the efficiency of the same three-level system working in the conventional two-bath model. We also study the same protocol for two coupled qubits and show that similar results can be obtained. The main result is to explain the mechanisms behind this phenomenon without invoking arguments related to entanglement or other properties from quantum theory, such as quantum coherence and discord, as was stated in some other works.

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Part I

Theoretical Background

Introduction

The understanding behind the notion of heat goes back to ancient times. Several attempts to explain its nature have been proposed since then, from phlogiston theory, caloric theory to mechanical theory of heat [1]. It was only during the industrial revolution that the heat theory advances began to be used for practical and useful applications, especially for the study of steam engines' performance. This was the beginning of a phenomenological theory that undoubtedly turns out to be one of the most successful theories in science's history - thermodynamics. Historically, thermodynamics adopted a different approach from other theories which gives a complete description of nature from a single particle system or even from a microscopic perspective. Among them we can cite classical mechanics that, for instance, can describe the dynamics of rigid bodies, electromagnetism which describes charged particles and its interactions through Maxwell's equations, and quantum mechanics with its own mathematical formulation to describe particles on their most fundamental level. All these theories can be expanded to a many particles case with no restriction within its formulation.

Thermodynamics, on the other hand, makes use of macroscopic parameters such as volume, pressure and temperature to explain the behavior of large systems - to the order of 10^{23} particles. Within this formulation, considering the amount of particles, there is no need, a priori, to access the internal description of each subsystem to be able to understand the behavior of the composed macro system. In order to understand this process in a more fundamental level, the advent of the atomic theory allowed a more precise description of thermodynamic phenomena from a microscopic perspective, considering the atomic dynamics and probability theory, giving rise to the statistical physics theory [2, 3, 4]. From this microscopic approach, statistical physics allows one to connect the microscopic world variables, which are constantly fluctuating due to its inherent chaos and randomness nature, by taking the average values of these variables in the limit of many particles system - thermodynamic limit. The result can be observed in terms of macroscopic variables. All of this can be done with no problem when one assumes that the system is always in thermal equilibrium.

For the last few decades, some attention has been given to non-equilibrium thermodynamics in microsystems. In such systems there is a need to take into account the thermal fluctuations, which will play an essential role in this new description, namely stochastic thermodynamics [5]. There are two remarkable fluctuation relations that make a connection between non-equilibrium process and thermodynamics quantities in equilibrium, namely Jarzynski's equality [6] and Crooks' relation [7]. It's natural then to wonder if the validity of thermodynamics with stochastic variables can be extended to the quantum regime. This question leads to a new emerg-

ing field that merges thermodynamics, a theory of many particles and degrees of freedom, and quantum mechanics, a theory of subatomic scale systems with a few degrees of freedom, into a new theory - quantum thermodynamics [8, 9, 10, 11].

Quantum thermodynamics aims not only to understand the thermodynamic behavior of macro-systems from the quantum dynamical perspective, but also to explore how and what quantum effects, if any, such as entanglement, any other non-classical correlations and quantum coherence, can affect thermodynamic processes [12, 13, 14, 15, 16, 17, 18, 19, 20]. The birth of quantum thermodynamics may be dated to 1959, when Scovil and Schulz-DuBios worked on a project connecting separated ideas from a new perspective, making an equivalence between a three-level maser system with the well established Carnot heat engine [21]. In their work, the amplified light was identified as being the work of the engine, while the heat was identified as being kinetic energy responsible for the population inversion generated by the heat baths. Later they published another work on Maser and Laser cooling [22, 23]. Since then, several different fields have helped with the development of this (still) emerging field.

As an interdisciplinary field, there are some approaches to explore phenomena from different perspectives, each one with its own insights. For example, the study of thermal machines are usually approached from quantum optics formalism [21, 23], many-body physics, fluctuation relations approaches [24, 25], resource theory [26, 27, 28], path integral approach [29], information theory approach [30], among others. This latter approach to quantum thermodynamics is based on the link between thermodynamics and information theory, which explores information acquired about the system to use as a resource for thermodynamics process. This idea was first proposed by J.C. Maxwell in his thought experiment, known now as Maxwell's Demon [31, 32, 33]. A more detailed analysis will be given in the next chapter.

From all of those branches, one of the main subjects that has already been extensively studied by the community is the study of the well-known and understood classical thermodynamic processes and their application in thermal machines [34, 35, 36], leading to a possible miniaturization of such engines to future technology. Besides quantum heat engines, there are several other applications of quantum thermodynamics, such as: quantum batteries [9, 37, 38, 39, 40, 41, 42, 43], absorption refrigerator [44, 45, 46, 47, 48, 49, 50, 51, 52], quantum thermometry [11, 53, 54], among others.

The structure of this dissertation goes as follows: In chapter 2, we briefly review the basic concepts of classical thermodynamics, like the concept of heat and work, the laws of thermodynamics and their counterpart in the quantum realm. We also show two important fluctuation theorems and present a little introduction to the information approach to thermodynamics in small systems, introducing the idea of the Maxwell's demon. In chapter 3, we review the concept and the basis of one important application of quantum thermodynamics, the quantum thermal machines. We first introduce the four basic thermodynamic processes, namely isothermal, isochoric, isobaric and adiabatic process and then we compare some differences between classical and quantum versions. Next we review two of the most important heat engines, both in classical and quantum regime, namely, Carnot and Otto cycles. The importance of the Carnot cycle is that it imposes a constraint to all other known cycles, stating an upper bound on the possible efficiency that an engine can reach. In the quantum case it is still valid as we will show. The Otto cycle has been daily used until these days. In this sense, the interest in optimizing the efficiency is not surprising. In this chapter we will describe the Otto cycle with more detail than the Carnot cycle, since we will use it later on our results. We also present a new kind of quantum Otto heat engine which was recently proposed in 2017 [55]. This engine makes use of the quantum measurement, instead of a hot heat source, in order to inject energy into the system, while there is only one true heat reservoir in the

setup. This kind of setup with quantum measurement is different from the Maxwell's demons-like application to quantum thermal machines as we will see. Finally, in chapter 4, we show our results based on the measurement-based quantum Otto heat engine for a three-level system and for a two qubit system as our working substance. In the last chapter we present the conclusions and future perspectives. In this analyses, we use the convention of $k_B = \mu_B = 1$. Thus, the other parameters, such J and B will have scale of energy.

Quantum Thermodynamics

2.1 Fundamental concepts

Unlike any microscopical system that can be completely defined classically by a Hamiltonian function or by a Hamiltonian operator for quantum systems, a thermodynamic system can be fully specified by state functions, like internal energy U and entropy S . These state functions are defined on the space of macrostates. In order to define a macrostate we need a complete set of independent state variables Γ_i , where $i = 1, 2, \dots, n$ and n is the total number of the macrovariables, which is much smaller than the number of microscopic variables for the system under consideration. Due to this lack of variables, the macroscopic variables do not fully describe the system properties, only the average values of them.

The macrostate variables can be of two kinds: extensive (X_i) or intensive variables (Y_i). As for the first ones, when the system's size changes, their values change as well by the same ratio, e.g., volume V , internal energy U , entropy S , and thus it must be an additive quantity. Intensive variables on the other hand remain the same no matter how much the system changes its size, e.g., pressure P , temperature T . There's a close relation between both quantities. In fact, for each extensive variable X_i there is a conjugate intensive variable Y_i . If a macrostate function is given only in terms of extensive variables, one can apply a coordinate transformation to get a new state function in terms of intensive variables. This process is called Legendre transformation [56, 57].

A process that takes an initial state function defined by some set of macrostate variables $X_i = \{x_1, x_2, \dots, x_n\}$ to another state function of $X'_i = \{x'_1, x'_2, \dots, x'_n\}$ through a sequence of changes is called a thermodynamic process. Such process can happen in a reversible or irreversible way, with the first one being exclusive for quasi-static processes where the system remains in equilibrium for whole time during the procedure. For instance, if a reversible process takes a state from point A to point B, one can take back the state from B to A by doing the inverse process. Equilibrium states are taken as a fundamental experimental fact. Any isolated system that has been disturbed in some way by the surrounding environment approaches the equilibrium state provided enough time (relaxation time). After reaching this state, it won't change until some interaction is made. In this sense, a process of a non-equilibrium system that evolves into an equilibrium state after its relaxation time is an example of irreversible process.

The way we can model these thermodynamic processes will depend on a number of factors. There are basically three types of models that a thermodynamic system can be presented: Isolated, closed and open. The first one means that the system under consideration has no interaction with the surrounding environment, no exchange of matter or energy is allowed. Certainly, this is just an

idealized model to describe a system, there is no such isolated system in nature. A closed system is one which can't exchange matter with the environment but it is able to exchange energy. An open system is one where every kind of exchange may occur.

The energy exchange that occurs in any thermodynamic processes can be one of two kinds: work and heat. The first one was of special interest back in the industrial revolution. Therefore, before we proceed to the laws that rule all thermodynamic processes, we introduce one definition which allow us to calculate the energy exchange contribution due to the work. In a thermodynamic process for a machine's cycles, work is both done on and by the working substance that is being used as a fuel to this engine. An useful heat engine is one from which more work can be extracted from the heat flux between the heat reservoirs than the work we need to invest in order to start the engine's cycle. We can define an infinitesimal amount of work in terms of the macrovariables, $W(\Gamma_i)$, as

$$\delta W = \sum_{i=1}^n \frac{\partial W}{\partial \Gamma_i} \Gamma_i, \quad (2.1.0.1)$$

where the notation δ indicates an infinitesimal change for which

$$\frac{\partial}{\partial \Gamma_j} \frac{\partial W}{\partial \Gamma_i} \neq \frac{\partial}{\partial \Gamma_i} \frac{\partial W}{\partial \Gamma_j}. \quad (2.1.0.2)$$

This quantity is not an exact differential and due to the fact that work is path dependent, i.e, depends on the process chosen to take a state from one point to another, the integral over a closed curve is not zero

$$\oint \delta W \neq 0. \quad (2.1.0.3)$$

It is possible to introduce an integrating factor for the work such that W becomes integrable. Furthermore, two non-integrable quantities may sum up to an integrable one, as we will see in the energy conservation law. Any function of state must be an integrable quantity.

2.2 The laws of thermodynamics

As a phenomenological theory thermodynamics follows a total of four laws, which paraphrase ordinary experience and observation of nature. The main focus of this axioms is the equilibrium state and the processes that transform one equilibrium state into another one.

2.2.1 Zeroth law of thermodynamics

The zeroth law defines an equilibrium state relatively to its surrounding environment. The most common statement of the zeroth law can be expressed as:

If two systems A and B are in thermal equilibrium with a third system C, then A and B are in thermal equilibrium with each other.

Equilibrium states are uniquely characterized by an equation of state. For many macroscopic systems, such equations are given in terms of volume V , temperature T and pressure P , in which two of them are independent,

$$f(V, P, T) = 0, \quad (2.2.1.1)$$

where $f(V, P, T)$ is characterized by the system under consideration. For instance, for an ideal gas Eq.(2.2.1.1) becomes $PV = Nk_B T$, where N is the number of particles and k_B is Boltzmann's constant.

2.2.2 First law of thermodynamics

From classical mechanics, one can derive the dynamics from the knowledge of the system's energy. We also know that for completely closed systems, the energy is conserved:

$$dU = 0. \quad (2.2.2.1)$$

The internal energy U may change due to some controllable external energy transfer, for instance, a change of volume, $dU^{ext} = -PdV$, or a change of magnetization, $dU^{ext} = \vec{B}d\vec{M}$ where \vec{B} is the magnetic field.

For a closed system, we may have one more contribution besides the work done by some external parameter. This contribution is due to the energy exchange with the environment, which we call heat Q . Thus we can write the first law of thermodynamics as

$$dU = \delta W + \delta Q, \quad (2.2.2.2)$$

where dU is an exact differential, although δW and δQ , variation of work and heat, respectively, are not exact differentials. Since dU is an exact differential, the change of the internal energy does not depend on which path was chosen. This makes sense, since we expect energy to be only dependent on the state of the system. As stated before, U is a state function

$$\oint dU = 0, \quad (2.2.2.3)$$

which is another form of energy conservation statement just like eq.(2.2.2.2).

2.2.3 Second law of thermodynamics

As we have seen above, the first law of thermodynamics tells us that all energy is conserved. The second law tells us more about the reversible and irreversible processes, specially about the latter one. There are some statements to define the second law which are equivalent. Two of the most known are formulations given by Clausius (1854) and Kelvin-Planck (1882). The first one can be written as:

It is impossible for heat to flow by itself from a lower temperature reservoir to a higher temperature reservoir. That is, heat transfer can only occur spontaneously in the direction of temperature decrease.

This means, for example, that we cannot construct a refrigerator that operates without any work input. The Kelvin-Planck statement can be read as:

It is impossible for a system to receive a given amount of heat from a higher temperature reservoir and to provide an equal amount of work output. A device which operates cyclically and converting heat to an equivalent energy transfer as work, without any waste into some heat sink, is impossible. Alternatively, a heat engine cannot have a thermal efficiency of 100%.

Just like the first law, which places the energy conservation restriction on how the processes must happen, the second law imposes some constraints as stated above. In fact, the second statement is even more restrict. The efficiency limit for a heat engine working between two reservoirs at different temperatures is given by the Carnot limit (That's the Carnot statement of the second law).

The two formulations are equivalent in the sense that if any device violates the Clausius statement, it also violates the Kelvin–Planck statement. Both the Clausius and the Kelvin–Planck formulation of the second law are negative statements, which impose constraints on how thermodynamic processes can happen. The second law of thermodynamics is based on experimental observations, as any other physical law, and it has not been contradicted so far.

Mathematically, the second law was first expressed by Clausius as

$$\oint \frac{\delta Q}{T} \leq 0 \quad (2.2.3.1)$$

where T is the temperature of the system during a cyclic process and the equality is achieved only for a quasi-static (reversible) process. So a new state function can be defined in terms of reversible and irreversible processes as $dS = \delta Q/T$, where S is called the entropy. One can integrate this function from a point A to B for a given T during a thermodynamic transformation and obtain

$$\Delta S \geq \int_A^B \frac{\delta Q}{T}, \quad (2.2.3.2)$$

where ΔS is the entropy variation between both points. Again the equality is only achieved if the process is taken reversibly, i.e., quasi-statically. If the process occurring from A to B is irreversible, then the entropy of the total system will increase. Any other effect in the entropy for irreversible processes is forbidden by the second law. An example of irreversible process is the free expansion of a gas. But, if the process is controlled by a gradual expansion or compression, it will not change the entropy, so it will be a reversible process. It is impossible to observe a reversible process in nature, they are a good idealization for processes where the system does not get considerably disturbed by the environment.

2.2.4 Third law of thermodynamics

The third law of thermodynamics, or the Nernst theorem, dictates that as closer to the absolute zero the temperature gets ($T \rightarrow 0$), the entropy change approaches zero as well:

$$\lim_{T \rightarrow 0} \Delta S = 0. \quad (2.2.4.1)$$

This affects some other properties, e.g., specific heat. So the system is described by its minimum energy state.

2.3 Quantum systems

In order to study how thermodynamic properties emerge from the quantum world, one must use the mathematical formulation of quantum mechanics and quantum statistical mechanics [58, 59]. The most basic task one may ask is how to write the energy conservation through the Hamiltonian description of quantum systems. In the following we will show how to obtain the first law of thermodynamics for quantum systems and how to associate the definitions of heat and work with these energy conservation laws.

2.3.1 Energy conservation

Let's consider a quantum system in a state given by the density matrix $\rho(t)$, with dynamics ruled by the Hamiltonian $\mathcal{H}(t)$. For any observable A , we have its average, for a certain $\rho(t)$, given by

$$\langle A \rangle = \text{Tr}[\rho(t)A]. \quad (2.3.1.1)$$

Since the Hamiltonian is the energy observable, we can identify the average energy of the system as

$$U = \langle \mathcal{H}(t) \rangle = \text{Tr}[\rho(t)\mathcal{H}(t)]. \quad (2.3.1.2)$$

Although eq.(2.3.1.2) is a simple equation, its evaluation may be more complex than we expect. In principle, the Hamiltonian above can be as simple as a free particle system or a more complex system with some interaction terms, which, sometimes, can be written as an effective Hamiltonian. For quantum open system, the dynamics will not be given by the Hamiltonian [60]. Since the system and the Hamiltonian vary on time, we may consider an infinitesimal variation on the internal energy and write it as

$$\begin{aligned} dU &= d\langle \mathcal{H}(t) \rangle = d\text{Tr}[\rho(t)\mathcal{H}(t)] \\ &= \text{Tr}[d\rho(t)\mathcal{H}(t)] + \text{Tr}[\rho(t)d\mathcal{H}(t)]. \end{aligned} \quad (2.3.1.3)$$

From eq.(2.3.1.3) one can associate the two terms on the right hand side as follows: the first term is the reconfiguration in the density matrix of the system due to some coupling interaction with the environment. In this sense, we can define this first term contribution as the average of heat, since it is an uncontrollable feature for the experimenter. The second term is the variation on the Hamiltonian due to the change in some external parameter, e.g, magnetic field, frequency, which an experimenter may have full control of as more precise his equipment is. Therefore, we can define this energy contribution as the average of work. This suggests a natural definition of average of heat and work first proposed by Robert Alicki [61]:

$$\langle \delta Q \rangle := \text{Tr}[d\rho(t)\mathcal{H}(t)] \quad \text{and} \quad \langle \delta W \rangle := \text{Tr}[\rho(t)d\mathcal{H}(t)]. \quad (2.3.1.4)$$

After identifying the terms above, we can write eq.(2.3.1.2) as the first law of thermodynamics for quantum systems in the same way we did in section (2.2):

$$\Delta U = \langle Q \rangle + \langle W \rangle, \quad (2.3.1.5)$$

where $\langle Q \rangle$ and $\langle W \rangle$ are given by

$$\langle Q \rangle = \int_0^\tau dt \text{Tr}[\dot{\rho}(t)\mathcal{H}(t)], \quad (2.3.1.6)$$

$$\langle W \rangle = \int_0^\tau dt \text{Tr}[\rho(t)\dot{\mathcal{H}}(t)]. \quad (2.3.1.7)$$

These integrals are taken over the thermodynamic process trajectory, which takes the system from $\rho(0)$ and $\mathcal{H}(0)$ to $\rho(\tau)$ and $\mathcal{H}(\tau)$, meaning that the path chosen matters for the quantification of work and heat. On the other hand, the internal energy only depends on the initial ($\rho(0), \mathcal{H}(0)$) and final ($\rho(\tau), \mathcal{H}(\tau)$) state of the system. This is in agreement with the previous notation of not exact differential for the heat and work and exact differential for the internal energy. Finally we can write eq.(2.3.1.5) as

$$\Delta U = \int_0^\tau dt \frac{d}{dt} \text{Tr}[\rho(t)\mathcal{H}(t)] = \langle Q \rangle + \langle W \rangle. \quad (2.3.1.8)$$

If one writes the Hamiltonian and the density matrix in the energy eigenvector basis, then eq.(2.3.1.3) can be written in a more explicit way. First, let us assume that the Hamiltonian belongs to a particular group of operators that posses eigenvectors that does not depend on any parameter. This assumption will be important for our results later. Now let the Hamiltonian be written in the energy basis and the density matrix as

$$\mathcal{H}(t) = \sum_n E_n(t) |n\rangle \langle n|, \quad (2.3.1.9)$$

and

$$\rho(t) = \sum_n P_n(t) |n\rangle \langle n| + \rho_{coh}(t), \quad (2.3.1.10)$$

where $E_n(t)$ and $|n\rangle$ are the eigenvalues and eigenvectors of the Hamiltonian, respectively. The density matrix is divided in two parts: the first one is the diagonal part, where $P_n(t)$ is the population and $\rho_{coh}(t)$ is the off-diagonal elements, also known as coherence terms. Then if we take the mean value in this basis, we get $U = \langle \mathcal{H}(t) \rangle = \sum_n E_n P_n$. For a small variation of the internal energy one gets

$$\begin{aligned} dU &= d \sum_n E_n(t) P_n(t) \\ &= \sum_n E_n(t) dP_n(t) + \sum_n P_n(t) dE_n(t) \\ &= \langle \delta Q \rangle + \langle \delta W \rangle, \end{aligned} \quad (2.3.1.11)$$

where one can identify the first term of the right hand side as the mean value of heat and the second one as the mean value of work. It is clear from this equation that the association of these quantities as heat and work makes sense. Work is the energy contribution that changes the eigenvalues of the system, when an external parameter is changed, and heat is the energy contribution that comes from the reconfiguration of the system after being disturbed by some interaction. If we consider a general eigenvector, i.e., any set of eigenvector that depends on some parameter, the Alicki's definition may present some problems [62].

Usually, these definitions are used when the interaction between the bath and the system under consideration is made until its complete thermalization. Then, it is detached from the bath

and evolves as a closed quantum system (unitary evolution) [63, 35, 36, 64, 65]. Other definitions were proposed when the system evolves as a quantum open system, considering interactions with the environment even after detaching from the bath [66]. It is worthy to mention that those are not the only definitions accepted in the literature. Another definition widely used is motivated by the Two Projective Measurement protocol (TPM) [67, 68, 69]. This protocol consists of defining work as the difference of energy of a given quantum system at the initial and final point of a certain process. The protocol can be described as follows:

1. Prepare your initial quantum state;
2. First energy projective measurement, $E(0)$;
3. Let it evolve from $\mathcal{H}(0) \rightarrow \mathcal{H}(\tau)$ while it is isolated from any environment;
4. Second energy projective measurement, $E(\tau)$.

In this sense, the work in a single cycle is defined as $W = E(\tau) - E(0)$ and the mean work will be given as an average over an ensemble of procedures. The work becomes a stochastic variable considering the non-deterministic property of the measurement process. In addition, the probability distribution will depend on both thermal fluctuations (step 2) and quantum fluctuations (steps 3 and 4). One of the reasons this definition has been used is due to the fact that it agrees with the quantum fluctuations theorems [67, 68, 69].

Despite the success of the TPM definition, it still has some problems. For instance, the validity of the work definition as the difference of the measured energies holds only for isolated systems. Besides that, this protocol does not take into account the invasive property of the measurement process when the initial state presents coherence in the energy basis, leading to a difference between the mean work calculated from an ensemble of realizations and the first law [70, 71].

As our intention in this dissertation is to study quantum heat engines, we must study all energy exchanges during the processes, i.e., in form of work and heat. Unfortunately, the TPM protocol does not provide any means to calculate the heat contribution. In this sense, the definitions eq.(2.3.1.7) and eq.(2.3.1.6) are taken as more intuitive and do not present the measurement problem to calculate the work and heat during a process. Thus, we will choose Alicki's definition to study quantum heat engines in the following chapters. In addition, for the chosen examples that we studied in chapters 4, due to the simplicity of the eigenvectors¹, the TPM protocol definition coincides with Alicki's definition of work.

2.3.2 Open quantum system approach

All the discussion above deals with closed quantum systems, when the system evolves unitarily after being detached from the bath. To study a more realistic quantum system, one needs to deal with the surrounding interaction due to the environment and other perturbations. Therefore, the Schrodinger equation must be replaced by a more general equation that may include these external interactions. Unlike closed quantum systems, open systems cannot be described by unitary evolutions. In many cases, the equation that describes a subsystem, $\rho(t)$, in contact with some environment is given by the Gorini-Kossakowski-Lindblad-Sudarshan, or just Lindblad equation [60, 72]:

¹By simplicity we mean that the eigenvectors does not have any dependence on some parameter.

$$\frac{d}{dt}\rho_s(t) = -i[\mathcal{H}(t), \rho_s(t)] + \sum_k \left[L_k \rho_s(t) L_k^\dagger - \frac{1}{2} L_k^\dagger L_k \rho_s(t) - \frac{1}{2} \rho_s(t) L_k L_k^\dagger \right], \quad (2.3.2.1)$$

which is also called master equation. In eq.(2.3.2.1), $\rho_s(t)$ is the reduced density matrix of the system of interest, $\mathcal{H}(t)$ is the Hamiltonian, $[\bullet, \bullet]$ is the commutator relation and L_k are the Lindblad operators. This equation is exclusive for the dynamics of the subsystem that we are interest in, the environment interaction is only described by the Lindblad operators, its dynamics does not matter. Mathematically, the dynamics is a completely positive trace-preserving operation. However, some restrictions are considered in the deduction of this kind of master equation. For instance, it obeys the Markovian property, which means that the dynamics is memoryless, it doesn't matter the past dynamics of the system to describe the future dynamics through eq.(2.3.2.1). Other approximations must be taken into account in order to derive this form of master equation, like Born approximation, which assumes that the environment and system interaction is weak, in the sense that the energy of the bare system's Hamiltonian (\mathcal{H}_s) is greater than the interaction energy of the bath-system Hamiltonian (\mathcal{H}_{int}): $\mathcal{H}_{int} \ll \mathcal{H}_s$. And secular approximation which involves discarding fast oscillating terms in the Markovian master equation approximation [73]. This approach is widely used to describe the interaction of quantum systems with reservoirs in quantum thermodynamics setups [11, 73, 74, 75, 76, 77, 78]

2.4 Fluctuation Theorems

In this section we will briefly show two important theorems that extend the second law of thermodynamics, which was at first formulated for systems at equilibrium, to non-equilibrium states and show that it will also hold in such cases. These theorems are known as the Jarzynski relation [6] and Crooks' fluctuation theorem [7]. Before we get into these theorems, we should look back at the second law of thermodynamics. As stated in section (2.2.3), this law sets a condition for entropy behavior over reversible and irreversible thermodynamic processes. If we rewrite the first law of thermodynamics with entropy definition, one gets

$$\begin{aligned} \Delta U &= \langle W \rangle + \langle Q \rangle \\ &\leq \langle W \rangle + T\Delta S, \end{aligned} \quad (2.4.0.1)$$

than we can define the following state function:

$$\langle W \rangle \geq \Delta U - T\Delta S \equiv \Delta F, \quad (2.4.0.2)$$

where ΔF is the variation of the Helmholtz free energy of the system (F), which is also a state function just like the entropy. From Clausius' inequality the second law constraints the total work that we need to do in order to perform a thermodynamic process as

$$\langle W_{in} \rangle \geq \Delta F, \quad (2.4.0.3)$$

where $\langle W_{in} \rangle$ is the work done on the system and ΔF can be interpreted as the available energy to be used as useful work. As already mentioned, work and heat are path dependent, so there is a path that maximizes the work done by the system.

2.4.1 Jarzynski equality

The thermodynamics framework is composed by many particle systems, where statistical mechanics is an essential tool to describe not only the probabilities of its dynamics but also the thermal fluctuations inherent to its own nature. In the quantum regime, not only the thermal fluctuation exists but there is also a quantum fluctuation due to the inherent randomness of nature. The second law of thermodynamic was originally developed to deal with systems in an equilibrium state. In 1997, Christopher Jarzynski presented a formulation of a specific fluctuation theorem for micro-systems that generalizes the second law statement for either systems in equilibrium or far away from equilibrium, and even for few particle systems (outside of the thermodynamic limit) [6].

Let's now consider a single particle assigned to a point, $x = (q, p)$, in the phase space, where q is any relevant coordinate that specifies the micro-state configuration and p is the corresponding canonical momentum. Consider also a probability density function, $P(x)$, that describes an ensemble of particles also in phase space. The particle is ruled by the Hamiltonian denoted as $\mathcal{H}(x, \lambda)$, where x is the point in the phase space in which the energy is evaluated and λ is the external parameter associated with the force acting on the particle. The system's state will evolve according to the variation in the external parameter, which may vary in time, $\lambda(t)$. Here we assume that the system is weakly coupled with a bath at the inverse temperature $\beta = 1/k_B T$, and that the time scale of the variation of the work parameter is taken to be shorter than the relaxation time. In this case, the dynamics can be described by the Liouville equation [10].

From a time period $t = 0$ until $t = \tau$, the variation of $\lambda(t)$ changes the system's state while it is couple from the bath. The external variation of $\lambda(t)$ is responsible for the work done on the system. This work and the heat absorbed by the system due to the change of the coordinates are defined similarly to Alicki's definition as:

$$W(x_\tau, \tau) := \int_0^\tau dt \frac{\partial \mathcal{H}(x_t, \lambda(t))}{\partial \lambda(t)} \dot{\lambda}(t), \quad (2.4.1.1)$$

$$Q(x_\tau, \tau) := \int_0^\tau dt \frac{\partial \mathcal{H}(x_t, \lambda(t))}{\partial x_t} \dot{x}_t, \quad (2.4.1.2)$$

where both $W(x_\tau, \tau)$ and $Q(x_\tau, \tau)$ are stochastic quantities that depend on the path taken by a single trajectory, x_t , followed by a particle during the interval $t \in [0, \tau]$. The energy change of the system is given by

$$W(x_\tau, \tau) + Q(x_\tau, \tau) = \mathcal{H}(x_\tau, \lambda(\tau)) - \mathcal{H}(x_0, \lambda(0)). \quad (2.4.1.3)$$

When the system is isolated from the bath, we may apply the Hamiltonian equations of motion², which are valid for closed systems, and one can obtain the following result:

$$Q(x_\tau, \tau)^{closed} = \int_0^\tau dt \left(\frac{\partial \mathcal{H}(x_t, \lambda(t))}{\partial q_t} \dot{q}_t + \frac{\partial \mathcal{H}(x_t, \lambda(t))}{\partial p_t} \dot{p}_t \right) = \int_0^\tau dt (-\dot{p}_t \dot{q}_t + \dot{q}_t \dot{p}_t) = 0 \quad (2.4.1.4)$$

$$W(x_\tau, \tau)^{closed} = \mathcal{H}(x_\tau, \lambda(\tau)) - \mathcal{H}(x_0, \lambda(0)). \quad (2.4.1.5)$$

²Hamiltonian equations of motion: $\frac{\partial \mathcal{H}}{\partial q} = -\dot{p}$ and $\frac{\partial \mathcal{H}}{\partial p} = \dot{q}$

So, all the system's energy changes during a closed system process is identified as work and no heat is exchanged, as expected for closed systems. This is the work done on the system for each single trajectory. For a mean value of the work, we must consider all possible trajectories available for a particle if we repeat the experiment many times, each time with the same initial state and bath, following the same protocol. With these considerations, one can evaluate the mean value of work as $\langle W_\tau \rangle = \int P_t(x_t) W(x_t, \tau) dD(x_t)$, where $P_t(x_t)$ is the probability density of a trajectory x_t and $dD(x_t)$ is the phase space integral over all trajectories [79]. But since we are considering closed systems, the trajectories will be fully determined by the initial point in the phase space due to its deterministic evolution from x_0 to x_τ . Thus for a particle starting from a phase space point, x_0 , it will present a initial trajectory probability density $P_0(x_0)$ and $dD(x_0) \rightarrow dx_0$ with a Jacobian determinant $dx_0/dx_\tau = 1$. Now we can rewrite the stochastic work for a closed system as

$$\begin{aligned} \langle W(x_\tau, \tau)^{closed} \rangle &= \int P_0(x_0) (\mathcal{H}(x_\tau, \lambda(\tau)) - \mathcal{H}(x_0, \lambda(0))) dx_0 \\ &= \int P_0(x_\tau) \mathcal{H}(x_\tau, \lambda(\tau)) \left| \frac{dx_0}{dx_\tau} \right| dx_\tau - \int P_0(x_0) \mathcal{H}(x_0, \lambda(0)) dx_0 = U_\tau - U_0. \end{aligned} \quad (2.4.1.6)$$

That means that the average work is just the difference of the average energies. Finally, Jarzynski proved that the average exponentiated work done on the system can be written as

$$\begin{aligned} \langle e^{-\beta W(x_\tau, \tau)^{closed}} \rangle &= \int P_0(x_0) e^{-\beta W(x_\tau, \tau)^{closed}} dx_0 \\ &= \int \frac{e^{-\beta \mathcal{H}(x_0, \lambda(0))}}{Z(0)} e^{-\beta (\mathcal{H}(x_\tau, \lambda(\tau)) - \mathcal{H}(x_0, \lambda(0)))} dx_0 \\ &= \frac{1}{Z(0)} \int e^{-\beta \mathcal{H}(x_\tau, \lambda(\tau))} \left| \frac{dx_0}{dx_\tau} \right| dx_\tau = \frac{Z(\tau)}{Z(0)} = e^{-\beta \Delta F}, \end{aligned} \quad (2.4.1.7)$$

where

$$Z(t) = \int dp \int dq e^{-\beta \mathcal{H}(x_t, \lambda(t))} \quad (2.4.1.8)$$

is the partition function. This is the famous Jarzynski equality, which holds for arbitrary non-equilibrium processes and that can be fully determined by equilibrium parameters contained in ΔF . Although we only considered a closed system, Jarzynski generalized his equality to open quantum systems [80]. This relation is of extreme importance in quantum thermodynamics, since it includes all the non-equilibrium moments of the physical state under consideration and also makes the second law more robust, generalizing it to non-equilibrium states. It can be seen by Jensen's inequality³ that the Jarzynski equality turns into the second law of thermodynamics in the form of eq.(2.4.0.2).

2.4.2 Crooks relation

Two years after Jarzynski's paper on his equality, Gavin Crooks presented in 1999 his work in which he compared the relation between the forward and reverse processes of the same protocol. As an example of such processes, imagine a cylinder filled up with some gas. The act of pushing and pulling the piston in order to compress and expand the gas inside it are the forward and backward processes for this specific case.

³ $\langle e^{-\beta W} \rangle \geq e^{-\beta \langle W \rangle}$

The setup for this theorem is similar to the Jarzynski equality. There must be a physical system in thermal equilibrium with at least one heat bath until the beginning of some protocol under consideration and an external parameter, initially at $\lambda(0)$, which is fully controllable by the experimenter. The external parameter is used to drive the system thermalized at Gibbs state, $\rho_0 = e^{-\beta\mathcal{H}(x_0, \lambda(0))} / Z(0)$, out of equilibrium until it reaches a final state ρ_τ , which is not necessarily an equilibrium state. The reverse protocol also starts with a thermalized state $\rho'_\tau = e^{-\beta\mathcal{H}(x_\tau, \lambda(\tau))} / Z(\tau)$ while the external parameter is changed from $\lambda(\tau)$ to $\lambda(0)$, until it reaches the state $\rho'(0)$, which also is not necessarily an equilibrium state. The states $\rho(0)$ and $\rho(\tau)$ from the forward protocol may not be the same states of the reverse protocol, $\rho'(0)$ and $\rho'(\tau)$. In the backward process we need to consider the time reversal operation, which takes $x(q, p) \rightarrow x(q, -p)$. If the Hamiltonian of the system possesses some parameter that is invariant under the time reversal operation, e.g. magnetic field, we must invert them.

Unlike Jarzynski's equality, Crooks' work focus on the work probability distribution of both forward and backward processes, which we denote as $P_F(W)$ and $P_B(W)$, respectively. We can write the forward work probability distribution as

$$P_F(+W) = \frac{1}{Z(0)} \int dq \int dp \delta(W(x_\tau, \tau)^{closed} - W_F) e^{-\beta\mathcal{H}(x_0, \lambda(0))}, \quad (2.4.2.1)$$

where $Z(0)$ is given by eq.(2.4.1.8), $\delta(\bullet)$ is the Dirac delta function, $W(x_\tau, \tau)^{closed}$ is the work given by eq.(2.4.1.5) and W_F is the work done in the forward process. The energy variation in this process is due to the external parameter variation during the protocol, while the system is coupled to the bath. So according to the first law of thermodynamics, the internal energy variation is associated with the work done during the process. Analogously to the forward process, we can define a work probability distribution for the backward process as

$$P_B(-W) = \frac{1}{Z(\tau)} \int dq \int d(-p) \delta(W(x'_\tau, \tau)^{closed} - W_B) e^{-\beta\mathcal{H}(x'_\tau, \lambda(\tau))}, \quad (2.4.2.2)$$

where now we must replace $x(q, p) \rightarrow x'(q, -p)$ in the partition function $Z(\tau)$ in eq.(2.4.1.8), in the $W(x'_\tau, \tau)^{closed}$ and in the Hamiltonian. The work done in the backward process is defined as W_B . Crooks realized that both eq.(2.4.2.1) and eq.(2.4.2.2) are connected and one can be determined by the other. This relation is now known as Crooks theorem:

$$P_B(-W) = P_F(+W) e^{-\beta(W-\Delta F)}, \quad (2.4.2.3)$$

where ΔF is the free energy difference between the equilibrium states at the moments $\lambda(0)$ and $\lambda(\tau)$. It is interesting to note that if we integrate eq.(2.4.2.3) over the forward work distribution, we get:

$$\int dW P_B(-W) = \int dW P_F(+W) e^{-\beta(W-\Delta F)} \quad (2.4.2.4)$$

$$1 = \langle e^{-\beta(W-\Delta F)} \rangle.$$

However, unlike the Jarzynski equality, which is valid for a more general scenario [81], Crooks' theorem is only valid for Markovian processes. These fluctuations relations have been extensively studied both in classical regime [82, 83, 84, 85, 86, 87, 88] and extended for quantum regime [67, 68, 89, 90]. There are also papers on the fluctuation relations with feedback control [79, 91, 92, 93, 94, 95, 96], which assumes a different setup that involves the Maxwell's demon, what we will discuss in the next section.

2.5 Information and Thermodynamics

In this section we will briefly mention another approach to the thermodynamics of small systems, which merge two independent fields, information theory and thermodynamics, into one research field - Information thermodynamics [38, 97]. The origin of this field can be associated with the thought experiment proposed by J.C. Maxwell in 1871, now known as Maxwell's Demon [31]. The basic idea behind this thought experiment was to test the limitation of the second law of thermodynamics, which Maxwell wished to demonstrate that it was a statistical principle that holds for almost every situation, but not an absolute statement for all physical possibilities. The central role in this idea was to use the information about the physical system and convert it into a form of work extraction. For this end, he imagined a tiny creature that could have access to some information that a human could not obtain through regular experimental techniques, and from the knowledge about the information the demon could use it to surpass the limits of the second law of thermodynamics.

An application of this result is the well known Szilard engine [98, 99], which presented a greater efficiency than the limits imposed by the maximum heat engine efficiency, the Carnot limit. In this sense, the second law was violated. Not until Landauer's work in 1962 the solution came to solve this apparent problem and reconcile both information theory and thermodynamics in a way in which the second law was no longer violated by the demon. This solution was proposed considering any information setup as a thermodynamic system with some memory, used to store information acquired by the demon, needing to be erased in order to make a complete cycle that ends in the same initial state that it was first started. In this sense, information can be used as a thermodynamic resource to extract work during a thermodynamic processes. However, there are some considerations about the validity of this idea that won't be discussed here [100].

2.5.1 Maxwell's demon

The birth of the tiny being goes back to 1871, when James Clerk Maxwell introduced his thought experiment in the end of his book, 'theory of heat' [32], in a section called 'Limitation of the second law of thermodynamics'. The name 'demon' was given by William Thomson (Lord Kelvin) [101]. It was the first relation between information theory and thermodynamics, even before the formalization of the former one in the science community, which had its first elements introduced in 1948 by Claude Shannon in his paper [102]. The role of this demon is to show that the second law of thermodynamics has only a statistical certainty, as we will show next.

The second law states that any closed system that cannot permit neither change of heat nor volume, with the same pressure and temperature everywhere inside the system's volume, cannot produce a gradient of temperature nor pressure without some external work applied. But if we imagine a tiny being that possesses special faculties, such as observe each single particle inside a container filled up with some kind of gas, it could be able to do something more than a regular experimenter that can only describe the average behavior of the particles of gas.

Let's consider a box filled up with some gas in which the molecules have the average velocity given by $\langle v \rangle$ and that is in thermal equilibrium with some heat bath at some temperature T . Now we place a partition in the middle of the box that has a little door, which can be controlled by the demon without producing any work. The demon's ability allows it to observe each molecule individually, so it can distinguish the faster particles, with greater velocity than the average ($v > \langle v \rangle$), from the slower ones ($v < \langle v \rangle$). As one can see in fig.(2.1), by controlling the door in the partition, the demon can decide to only open the door when it observes the faster molecules (red points)

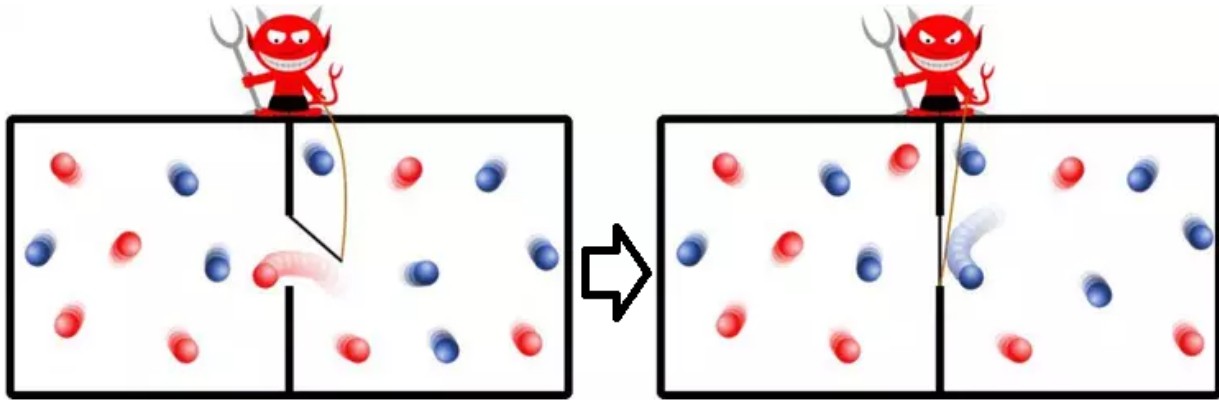


Figure 2.1: Maxwell's demon acting on molecules of some gas with average velocity given by $\langle v \rangle$. By controlling a little door, it lets the faster molecules (red) go from the right side to the left side of the box and slower ones (blue) from left to right, creating a gradient of temperature, which enables the extraction of work. [103]

going from the right to the left side of the box and the slower ones (blue points) the other way around. After a long time, the velocity distribution won't be described by the Maxwell-Boltzmann distribution, so the system won't be an equilibrium state anymore. At the same time, the left side will be filled up with faster particles and the right side with the slower ones. In this sense, the left side will be hotter, due to the kinetic energy of the molecules, than the right side, which we will call the colder side. If we keep the door closed, there is a way of use this temperature gradient to extract work. Therefore, work can be extracted from a system in contact with a single heat bath by exploiting the information knowledge acquired about the velocities of each molecule of gas, which only the demon has access. This kind of demon is called temperature demon. There could be also a 'less smart' demon which can operate in a single temperature system and generate a difference in pressure. Next we will show how this so-called pressure demon will be exploited in the famous engine designed by Szilard.

2.5.2 Szilard engine

In 1929, 58 years after the birth of Maxwell's demon, the physicist Leo Szilard brought to light a simple, but controversial, application of the demon's abilities [104]. He imagined a cylinder of volume V , which is all available for a one-molecule gas that we will consider as our working substance. In fig.(2.2), one can observe a four step process which describes all stages of the Szilard engine. Let's describe each one as following:

- (a) This first step consists in placing a mobile partition in the middle of the box of volume V , exactly like the Maxwell's thought experiment described in section (2.5.1). In doing so, the single molecule gas will be trapped in one of the two sides of the box of volume $V/2$.
- (b) This is the most important step of this setup. In this process we allow the demon to be part of the system in such a way that only it can make a measurement in the fluid in order to determine in which of the two chambers the molecule is in and records the result. In this example, the molecule is trapped in the right side of the box.
- (c) After knowing the side of the box where the particle is captured, we use this result to choose the same side to connect a system of pulley and rope coupled to some object in order to transform

the knowledge acquired into some form of work. This work must be done in a reversible way, the object should move continuously as the particle makes pressure in the mobile partition.

- (d) In this final step, we put the cylinder in contact with some heat bath at constant temperature T . In this way, all the heat transfer from the bath to the molecule will be entirely converted into work, which will raise the object as long the molecule moves the partition until the end of the box. When the partition reaches the end of the box, then the system apparently comes back to the initial state, with the molecule moving along the entire volume V .

The controversial part of this engine is found at the stage (d). In this step all the heat transferred from the heat bath to the particle is converted into work, $Q = W$, and then the system comes back to the same initial state. However, if we look at the entire system, gas and heat bath, one can note that the gas came back to its initial state, but the heat bath just transferred heat to the particle and had its entropy decrease by a certain amount, with no other effect. This apparently violates the second law in the end of a cyclic process. The work done in this process is given by

$$\begin{aligned} W &= k_B T \int_{V/2}^V \frac{1}{V'} dV' \\ &= k_B T \ln 2. \end{aligned} \tag{2.5.2.1}$$

This work could only be extracted because the statistical fluctuations are not negligible for this kind of situation. If there was a large number of particles in both sides of the box, the statistical fluctuations would be harder to be used as a resource, and it could not be so easy to detect some considerable difference in pressure from both sides of the box. Szilard tried to recover the second law by explaining that the act of measuring the position of the particle produces the missing extra entropy, so this was the cost to be paid in order to extract that amount of work. But in the end, it was unclear whether the real cost came from the measurement act, the fact that the result of the measurement should be stored or from the erasing of the information. This problem was discussed and solved by other papers which will be briefly presented next.

2.5.3 Landauer's principle

As exposed above, the Maxwell's demon apparently extracts work from a single constant temperature heat bath as long as it is able to make a measurement on the system's microscopic degrees of freedom, then take the next step depending on the result. The fact that the next step depends on the result of the measurement implies that the demon must store the information acquired in this process for future application; it is called the demon's memory. In this sense, the cycle of Szilard's engine is not fully complete until the demon's memory state comes back to its initial value as well as the gas molecule and the heat bath. This is the erasure process of the information stored in the demon's memory. Neither Maxwell nor Szilard considered the memory as a thermodynamic cost in the cycle. Actually Szilard thought that the act of measuring was responsible for producing the extra entropy necessary to hold the second law of thermodynamics.

In 1951, Brillouin failed in his attempt to resolve the Maxwell's demon paradox [106], when he tried to justify the extra entropy on the measurement process. It was only in 1962 that Landauer analyzed this question more carefully and realized that it wasn't as simple as Szilard and Brillouin assumed [107]. While Landauer was working for IBM, studying if it was possible to do irreversible processes in computation tasks without energy dissipation, he argued that it was impossible to do

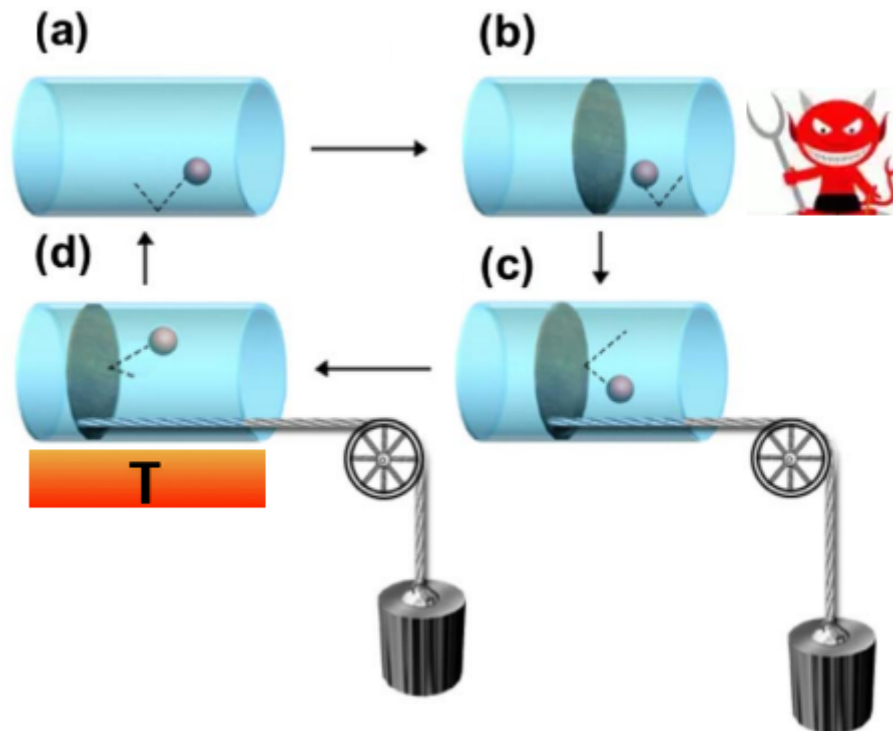


Figure 2.2: Szilard engine demonstrated in its four steps process. Process (a) \rightarrow (b): the demon makes a measurement and finds out the position of the particle and records the result as a bit of information. Process (b) \rightarrow (c): The demon uses the information to prepare a system which allow it to convert the information in some work form. Process (c) \rightarrow (d): work is extracted from the single molecule gas at constant temperature of a heat bath, by moving the partition until the end of the box. Process (d) \rightarrow (a): The system apparently comes back to its initial state. Figure adapted from [105]

so, because there is a minimum amount of energy necessary to erase a bit of information. His work states that to erase one classical bit of information⁴ from the memory, it is necessary to release at least $k_B T \ln 2$ of heat to the environment.

⁴One bit of information = $\ln 2$ nat. The nat is the 'natural' unit of information.

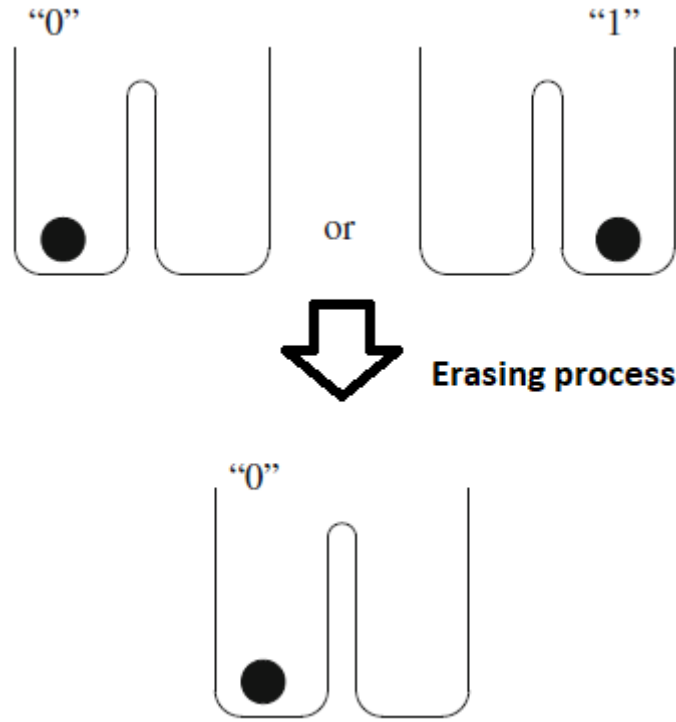


Figure 2.3: Landauer's principle representation. The particle is trapped in either one of the wells, after the erasure of the memory, the particle always comes back to the left well. Figure adapted from [30].

Landauer's principle can be understood as follows. After the measurement, there is at least one bit of information stored in the memory, which is equal to $\ln 2$ nat. Let's represent the two possible outcomes of the measurement process in some two level system by "0" and "1", the classical bits representation. If the system is a particle trapped in one of two possible wells, the "0" bit represents the left well and the "1" bit represents the right well, as shown in fig.(2.3). The entropy associated to the information storage is equal to $k_B \ln 2$, and after the erasure process, the memory is always reset to the "0" state. This erasing causes a decrease in the demon's memory entropy which, according to the second law, is accompanied by some heat dissipation for the environment.

The minimum cost of energy dissipation in erasing a bit of information imposed by Landauer's principle is given by

$$\langle W_{min} \rangle = k_B T \ln 2, \quad (2.5.3.1)$$

which is the minimum work for erasing a bit of information and is exactly the same value of the work extracted by the demon during a cycle of the Szilard engine. So the net work is zero, in agreement with the second law. In 1982, Bennett wrote a paper where he gave an example that proves how Brillouin's argument was wrong and matches the Landauer's principle [108].

In sum, in the previous and the present chapters we briefly reviewed the basic concepts of classical and quantum thermodynamics. In the following part of this work, we will present one of the most important applications of thermodynamics - thermal engines. For this purpose, we will use the Alicki's definition of work and heat given by eq.(2.3.1.6) and eq.(2.3.1.7). After this discussion, we will apply these ideas to two examples, namely a qutrit system and a two qubit system as the working substance of the heat engine.

Quantum Thermal Machines

Quantum thermodynamics is still in its initial development, with a lot yet to be learned about the thermodynamic behavior emerging from small systems, with just a few particles, that obey quantum mechanics. Anyhow, scientists explore all possible paths in this emerging field, from theoretical point of view, trying to understand the most fundamental level, to applied researches, to be used in future micro-technology.

One of the main applications of classical thermodynamics is the thermal heat engines, which extract useful work from thermal energy baths. In this chapter we will discuss a basic and intensively studied application of quantum thermodynamics which is widely explored: quantum thermal machines, quantum counterpart of the standard classical heat engines. The first work on this subject goes back to 1959, when H. E. D. Scovil and E. O. Schulz-DuBois studied how a three-level system could be used to simulate a heat engine [21]. In their paper, they proposed a prototype of heat engine by using a three-level maser system as a thermal machine, where the fundamental difference between it and some regular 'classical' heat engine lies on the energy spectrum, which is continuous in the classical case. They showed that the efficiency of such micro-engine is upper bounded by the Carnot limit, as well as any other classical heat engine. In 1979, Robert Alicki presented his definition of heat and work for quantum systems [61], already shown in chapter 2 in eq.(2.3.1.6) and eq.(2.3.1.7), which are widely accepted and used by the community.

In the last few years there has been an enormous amount of work based on the study of thermal machines' efficiency with quantum systems as the working substance [35, 36, 34, 109, 110, 111]. The main idea of using quantum substance, e.g. single or coupled qubits, quantum harmonic oscillator, among others, is to explore intrinsic properties of quantum mechanics, such as entanglement and quantum coherence, to boost the efficiency over the classical limits obtained by non-quantum matter. The most common design of quantum heat engines consists in replacing the classical working substance for a quantum one instead, coupled to classical thermal reservoirs. But in doing so, it is not clear if there is some advantage in building this kind of machines over the classical and well understood ones [13, 14, 16, 15, 17, 18].

The efficiency of any machine will depend on the thermodynamic process involved in the heat engine cycle. For each kind of sequence of thermodynamic process set, there will be a different efficiency associated to it. The general formula for the efficiency is given by the ratio of total net useful work done by the system and the heat transferred by the heat bath into the system:

$$\eta = \frac{\langle W_{net} \rangle}{\langle Q_h \rangle}. \quad (3.0.0.1)$$

It is well known from standard thermodynamics that as the efficiency approaches to the maximum value, the power output also approaches to zero as the process is quasi-static. In 1975, F. L. Curzon and B. Ahlborn studied the Carnot cycle's efficiency working between two heat baths at different temperatures, cold T_c and hot T_h , at maximum output power. The efficiency obtained is given by

$$\eta_{C-A} = 1 - \sqrt{\frac{T_c}{T_h}}, \quad (3.0.0.2)$$

which is the Curzon-Ahlborn efficiency [112]. This equation is changed if one changes the constraints used by them in their work. Even though this result is also obtained by a classical physical system, the quantum version is also valid [113].

For the rest of this chapter we will present the basic thermodynamic processes which will characterize an engine cycle and then show some of the most important and known cycles using some quantum system as working substance. Next we will show a new kind of quantum heat engine which uses quantum measurements in order to provide energy to the system and then extract some useful work, which will be used in the next chapter as part of our results.

3.1 Basic thermodynamic processes

Before we explain how to build a quantum version of a thermal machine for some of the most known classical cycles, first we need to recall the most common thermodynamic processes that are fundamental to these engines. In this section we will briefly review the basic processes, namely isothermal, isochoric, adiabatic and isobaric ones. For all processes that will be presented here, we consider work and heat as defined in chapter 2 by eq.(2.3.1.11). Some attention will be given to the differences between the classical and quantum versions. It is also worthy to remember that both work and heat contributions can be originated from external or internal degrees of freedom of the system. For instance, we can extract work from the spin degree of freedom of a quantum system or from an external degree of freedom, like position. Now, allow us to begin the description of each process, starting by the isothermal one.

- **Isothermal process:** The classical isothermal process consists of exchanging work and heat while keeping the temperature constant. Let's consider, for instance, a cylinder coupled to a piston filled up with a classical ideal gas ruled by the equation of state given by $PV = Nk_B T$. If the system is in thermal equilibrium at some constant temperature T , we can slowly push or pull the piston without changing the temperature of the gas. This process is called isothermal compression and expansion, respectively. The volume variation during this process will be responsible for the work production according to: $W = -Nk_B T \int_{V_i}^{V_f} (1/V) dV$, where V_i (V_f) is the initial (final) volume.

Before we explain the quantum extension of the isothermal process, we will show how temperature can be defined for quantum systems. Consider a simple two-level system, for instance a qubit, which has a ground and excited states, $|g\rangle$ and $|e\rangle$ respectively, and an energy gap $\Delta = E_e - E_g$ between them. In an isothermal process, there must be a ratio between the occupation probabilities of the excited state P_e and ground state P_g , with a normalization condition $P_g + P_e = 1$, that satisfies the Boltzmann distribution. We can write the ratio between both probabilities as

$$r = \frac{P_e}{P_g} = e^{-\beta\Delta}, \quad (3.1.0.1)$$

where $\beta = 1/k_B T$, k_B is the Boltzmann constant and the temperature T . Then, one can define an effective temperature to the system under consideration as

$$T_{eff} = \frac{1}{k_B \beta_{eff}} = \frac{\Delta}{k_B \left(\ln \frac{P_g}{P_e} \right)^{-1}}. \quad (3.1.0.2)$$

This is a simple task to accomplish for a two-level system as long as the energy levels and occupation probabilities are known. The problem with effective temperature arises when one is dealing with any system with more than two levels. Even for a simple three-level system one could need to define an effective temperature for each subset of energy gaps between the energy levels [35].

Now let's extend this process to the quantum regime. Consider a single particle in contact with a heat bath at some constant temperature T , e.g, a particle trapped in a potential energy well. In order to perform an isothermal process, this particle should be able to exchange heat with the bath and perform some work. For a particle inside a box, for example, we can achieve this process by slowly changing the size of the box. To remain in equilibrium with the thermal bath at every instant, the occupation probabilities and energy gaps should change simultaneously, exchanging heat and performing work, respectively, according to eq.(2.3.1.11).

- **Isochoric process:** This process is very similar to both classical and quantum regime. In the classical case the volume V is kept constant, while the constant quantity in the quantum regime is the energy E . Consider once again an ideal gas inside a closed cylinder of volume V . The isochoric process is the one where the cylinder is put in contact with some heat source while the pressure changes due to the heating. Since the volume does not change, no work is done in this process ($W = 0$).

While the pressure P and the temperature T change in the classical regime, in the quantum regime the occupation probability P_n is the quantity that changes. Thus, the associated effective temperature and the entropy changes as well. From these physical quantities we can see that heat will be exchanged between the working substance and the heat bath, but no work is done since the volume and energy levels are maintained constant in the classical and quantum regime, respectively. There may be cases where we can associate the energy with the volume, making the classical and quantum isochoric process even more similar. Consider, for instance, a particle in a three dimensions box with all sides equal to L . The particle's energy is given by

$$E = \frac{\pi^2 \hbar^2 (n_x^2 + n_y^2 + n_z^2)}{2mL^2}, \quad (3.1.0.3)$$

where m is the mass of the particle. In this sense, we can associate the volume with the energy. No work will be done while the volume, and so the energy, doesn't change. Fig.(3.1) shows a generic scheme diagram of a multilevel system during an isobaric process. The left column is the initial state of the system with energies given by E_n^h with their respective population P_n^h . After the isochoric process, the population of each level changes while the energy remains the same.

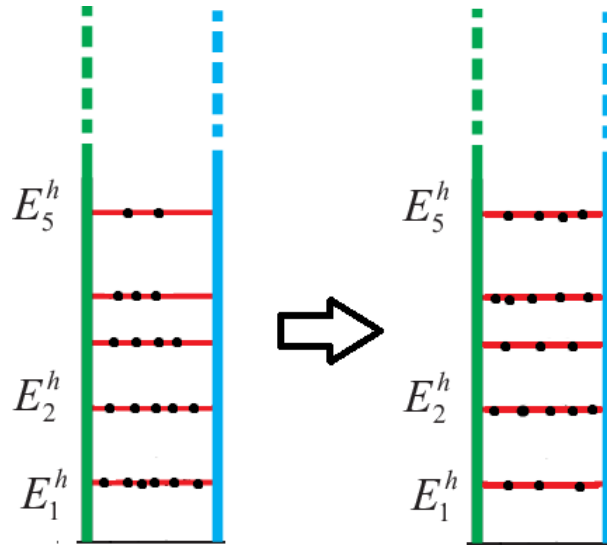


Figure 3.1: Isobaric process for a generic multilevel quantum system. Figure adapted from [35].

- **Isobaric process:** In classical systems the isobaric process is the one in which the pressure P is maintained constant during a quasi-static process. By quasi-static we mean that the time that the system takes to thermalize with the heat bath (relaxation time) is much smaller than the time to control the volume of the system. Let's take a classical ideal gas once again. In order to successfully realize an isobaric process, the temperature and the volume must vary in such way that $V \propto T$, ensuring that the pressure remains constant. For example, the isobaric process for an ideal gas inside a cylinder with a piston can be realized when the gas pressure is in equilibrium with the external pressure produced by the piston and the environment pressure. The work done in this process is given by $W = -P\Delta V$.

However, in quantum mechanics there is not a straightforward way to control the temperature in the same way that can be done in classical regime. There is a lack of some equation of state for quantum systems of few particles. To analyze this problem, we need to define pressure in quantum theory in terms of generalized coordinates.

Let's consider the first law of thermodynamics with generalized coordinates: $dU = \delta Q + \delta W = TdS + \sum_n Y_n dy_n$, where Y_n is the generalized force associated with the generalized coordinate y_n by the relation

$$Y_n = -\frac{\delta W}{dy_n}. \quad (3.1.0.4)$$

If we consider the volume V as the generalized coordinate, we recover the pressure as the generalized force. Using this same idea to define force in quantum mechanics, we can write it as

$$\mathcal{F} = -\frac{\delta W}{dL} = -\sum_n P_n \frac{dE_n}{dL}, \quad (3.1.0.5)$$

where L is the generalized coordinate associated with the force \mathcal{F} . From this equation we can, for instance, find the force of the particle acting on the walls of the three dimensional box presented above in eq.(3.1.0.3). This definition is general and does not depend on the system's state. But if the state is in equilibrium, there is a more straightforward way to get at the same result. Consider a system in thermal equilibrium with occupation probabilities

given by $P_n = e^{-\beta E_n} / Z$, where $Z = \sum_n e^{-\beta E_n}$. We can write the force starting from the free energy of the system, $F = -(1/\beta) \ln Z$:

$$\begin{aligned} -\left(\frac{\partial F}{\partial L}\right)_T &= \frac{1}{\beta} \left(\frac{\partial \ln Z}{\partial L}\right)_T \\ &= \frac{1}{\beta Z} \frac{\partial}{\partial L} \sum_n e^{-\beta E_n} = - \sum_n \left(\frac{e^{-\beta E_n}}{Z}\right) \frac{\partial E_n}{\partial L} \\ &= - \sum_n P_n \frac{dE_n}{dL} = \mathcal{F}. \end{aligned} \quad (3.1.0.6)$$

In the quantum regime, there won't always be an equation of state for every quantum system with a classical analogue. But the closest similar results to compare are the classical ideal gas and a single particle inside a one dimension box, where the pressure on the box's walls is given by

$$\mathcal{F} = \frac{1}{\beta L}, \quad (3.1.0.7)$$

where L is the length of the box. So, eq.(3.1.0.7) can be written as $\mathcal{F}L = k_B T$ as analogous to $PV = Nk_B T$. Thus, for a particle inside a one dimension box, the length of the box L should change proportionally to the inverse temperature β in order to keep the generalized force constant. For other quantum systems, there will be more complex equations of state-like. Other cases can be found in [35].

- **Adiabatic process:** Historically, the classical and quantum adiabatic processes have different origins. The classical adiabaticity, or thermodynamic adiabaticity, can be achieved by performing either very slowly (perfect insulation) or very fast processes (car's engine), without changing heat with the environment ($\delta Q = 0$). This process is widely used daily.

In quantum theory, the necessary condition to perform a successfully adiabatic process is that one must slowly disturb the system under consideration in order to avoid any excitations of the occupation probabilities. This condition is known as the quantum adiabatic theorem [114], which states that in order to perform a quantum adiabatic process, the change in the system must be done extremely slowly, proportional to the inverse of the energy gap, without changing its state. In doing so, the populations will remain constant, $dP_n = 0$.

While the classical adiabatic process deals with thermodynamic processes, the quantum one don't necessarily does. In this sense, the quantum adiabatic process can be viewed as a subclass of a classical adiabatic process when it is possible to associate the slow change in the system's Hamiltonian with some thermodynamic process. For instance, if one perform a quantum adiabatic process, where there is no population excitation, according to eq.(2.3.1.11), there won't be any generation of heat, $\langle \delta Q \rangle = 0$. The total energy exchange done during this process is identified as work energy contribution.

In table 3.1 we show a little review of the processes presented above with the crucial difference between the classical and quantum version.

	Isothermal	Isochoric	Isobaric	Adiabatic
Classical	Heat exchange Work done Fix: U, T Var: P, V, S	Heat exchange No work done Fix: V Var: P, T, S	Heat exchange Work done Fix: P Var: V, T, S	No heat exchange Work done Fix: S Var: P, V, T
Quantum	Heat exchange Work done Fix: T Var: U, E_n, P_n, S	Heat exchange No work done Fix: E_n Var: P_n, T, S	Heat exchange Work done Fix: \mathcal{F} Var: T, E_n, P_n	No heat exchange Work done Fix: P_n Var: T, E_n

Table 3.1: The four basic classical and quantum thermodynamic processes and their respective fixed ('fix') and variable ('var') parameters.

3.2 Quantum cycles

After a brief review of each one of the fundamental thermodynamic processes, we will apply them to the study of quantum thermal machines and see how they can be used in order to extract work from a quantum system. There are several heat engines in the literature, such as Carnot cycle, Brayton cycle, Diesel cycle and Otto cycle. Here we will present two of the most important ones, the Carnot cycle and the Otto cycle. All these cycles belong to a class of engines known as four-stroke engines, in which each stroke is a time branch where a certain process is done, for instance, any of the four processes presented above in section 3.1. The simplest example of a four-stroke engine is the Otto cycle, which will receive a special attention later in this chapter and the next one, because the work done by/on the system and heat exchange are produced separately, each one in a different stroke. Fig.(3.2a) shows each process during the Otto cycle on a single two-level system: The first stroke is the thermalization of the two-level system with a hot heat bath at some temperature T_h where heat exchange happens by changing the population of each energy level and is given by $Q_h = \langle E_2 \rangle - \langle E_1 \rangle$. Next, work is done by the system by decreasing the energy level gap while work is done on the system by expanding the energy level gap. The middle step, between both work strokes, is the thermalization with the cold heat bath at temperature T_c , where the heat is given by $Q_c = \langle E_4 \rangle - \langle E_3 \rangle$. To keep the validity of the first law, we must get $Q_h + Q_c + W_I + W_{II} = 0$.

Fig.(3.2b) shows a two-stroke engine. This engine is built into two parts: The first stroke involves the contact of a single particle coupled with a hot heat bath and another particle coupled with a cold heat bath. It is important that no interaction is being made between them while they are coupled to their own heat baths. The second stroke is the process of uncoupling the particles from the heat baths and then put them in contact with each other. As they undergo this evolution, some energy is converted into extracted work. The last kind of heat engine is presented by the continuous engine shown in fig.(3.2c). This study was first done in references [21] and then [116]. In this engine the baths and the external interaction are in continuously contact with the system.

3.2.1 Carnot cycle

The classical Carnot cycle is already well known and is the upper bound limit for every kind of classical heat engines' efficiency. In this section we will study the quantum counterpart of Carnot cycle and its properties. Just like the classical case, the quantum Carnot cycle is based on the same four-strokes, being them two quantum isothermal and two quantum adiabatic processes.

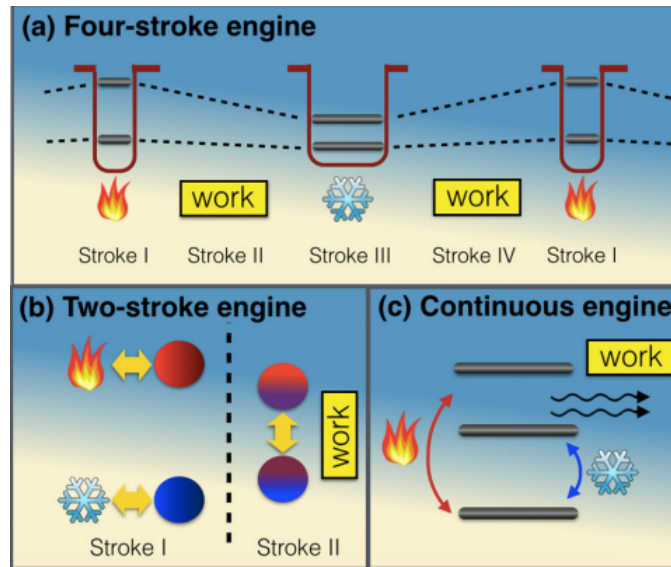


Figure 3.2: (a) A four-stroke engine represented for a two-level quantum system. (b) Two-stroke engine with two particle system as working substance. (c) Continuous engine with a three-level system as the working substance. Figure taken from [115].

We show in fig.(3.3) both classical and quantum cycles with their strokes. Fig.(3.3a) is a P-V diagram for an ideal gas during a Carnot cycle, where the processes $A \rightarrow B$ and $C \rightarrow D$ are the isothermal expansion and compression of the gas, respectively, at temperatures T_h and T_c . Processes $B \rightarrow C$ and $D \rightarrow A$ are adiabatic strokes, where the work is done on and extracted from the system. The four steps are the followings:

- **Isothermal (hot):** The system is coupled to a hot heat bath and absorbs heat from it.
- **Adiabatic expansion:** While the quantum substance is uncoupled from any heat bath the external parameter is changed from λ_i to λ_f . In this step work is done by the system due to the change in the energy levels and entropy is conserved.
- **Isothermal (cold):** The system is coupled to a cold heat bath at the temperature T_c . The system transfers heat to the bath in this process.
- **Adiabatic compression:** The external parameter is taken back from λ_f to λ_i while it is not in contact with any heat bath. Work is done on the system.

In fig.(3.4) the Carnot cycle is represented by a schematic picture for a many-level energy system. Process 1 is the heat absorption from the hot bath, that happens between time $\tau = 0$ and $\tau = \tau_1$, where the population changes during the isothermal process. Process 2, from τ_1 and τ_2 , is the adiabatic expansion, where work is done by the system. Step 3, τ_2 and τ_3 , is another isothermal process with a cold heat bath, where the system exchanges heat with the reservoir. Finally the fourth and final step, τ_3 and τ_4 , is the adiabatic compression, where work is done on the system.

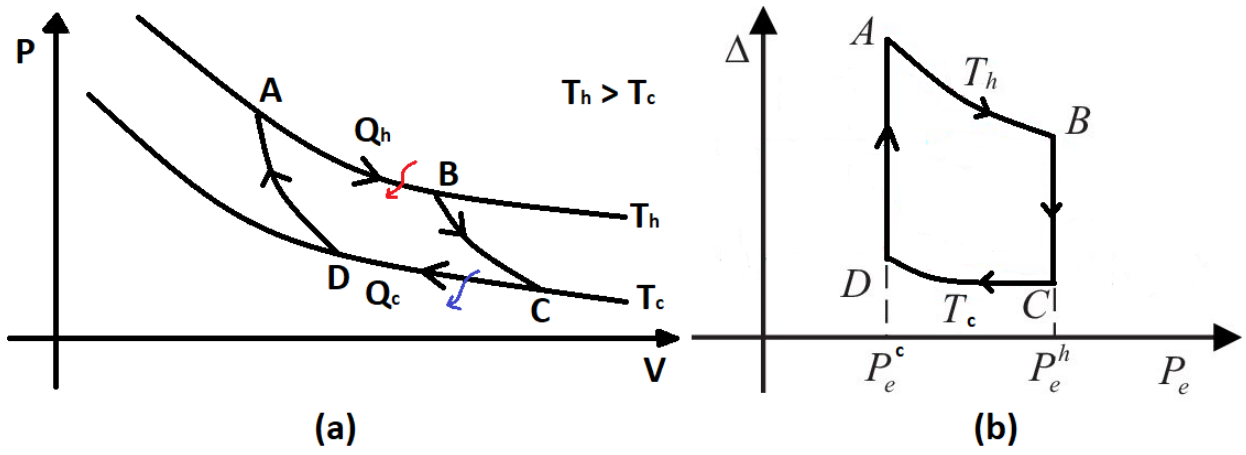


Figure 3.3: (a) Classical Carnot cycle represented in a pressure-volume diagram for an ideal gas with two isothermal processes (A to B and C to D) and adiabatic processes (B to C and D to A). (b) Quantum Carnot heat engine for a two-level system with Δ being the energy gap between them and P_e the occupation probability of the excited state.

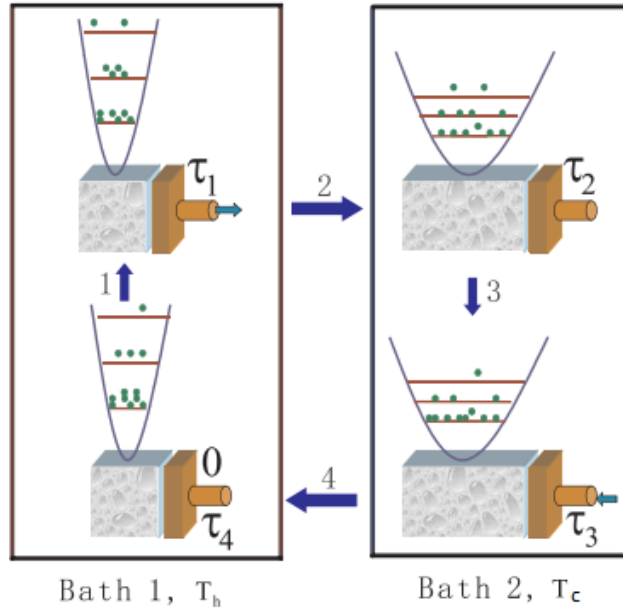


Figure 3.4: Schematic representation of Carnot engine with two adiabatic and two isothermal strokes. Figure taken from [115].

Let's now calculate the heat and work done in one cycle for a two-level system. The heat exchanged during the isothermal strokes can be calculated from the relation $dQ = TdS$. The absorbed and released heat are given by

$$Q_h = [S(B) - S(A)]T_h, \quad (3.2.1.1)$$

$$Q_c = [S(D) - S(C)]T_c, \quad (3.2.1.2)$$

where $S(x) = -k_B \sum_i P(X) \ln P(X)$ is the Shannon entropy, $X = A, B, C, D$ and $P(X)$ is the occupation probability. From fig.(3.3) we can see that $P(A) = P(D)$ and $P(B) = P(C)$, which implies $S(A) = S(D)$ and $S(B) = S(C)$. The work can be obtained from the above equations as

$$\begin{aligned}
 W &= -(Q_h + Q_c) \\
 &= -(T_h - T_c)(S(B) - S(A)).
 \end{aligned}
 \tag{3.2.1.3}$$

Then the efficiency of a quantum Carnot engine is give by

$$\eta_C = -\frac{W}{Q_h} = 1 - \frac{T_c}{T_h}.
 \tag{3.2.1.4}$$

This efficiency has exactly the same form both for the classical and quantum cycles. The ratio of the temperatures also plays an important role in the condition for the cycle to work reversibly, as a heat engine is supposed to be:

$$E_n(C) - E_m(C) = \frac{T_c}{T_h} [E_n(B) - E_m(B)].
 \tag{3.2.1.5}$$

This condition means that all the energy gaps must change at the same rate during the adiabatic process, where E_i is the energy of the quantum state $|i\rangle$. Eq.(3.2.1.5) is a sufficient and necessary condition to perform a reversible quantum Carnot cycle [35].

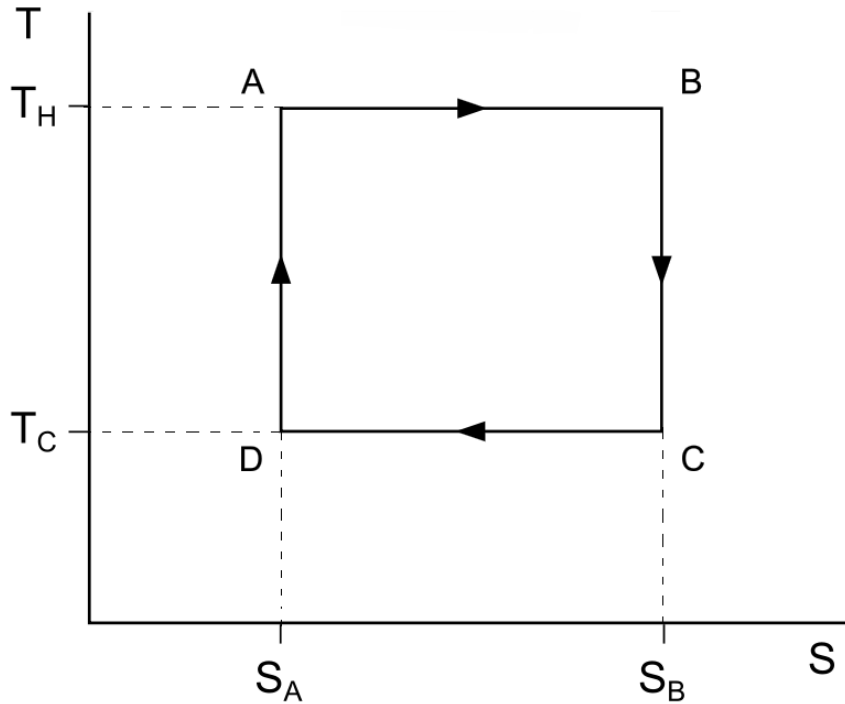


Figure 3.5: $T - S$ diagram for both classical and quantum Carnot cycle. This diagram is based on a two-level system and an ideal gas for quantum and classical cycle, respectively.

3.2.2 Otto cycle

In this section we will explore the heat engine which is widely used as an internal combustion engine in automobiles, the Otto cycle, named after the German engineer Nikolaus Otto. This has been extensively studied in the literature [34, 117, 118, 119, 120, 121]. As its classical counterpart, the quantum Otto engine consists of two quantum isochoric and two quantum adiabatic

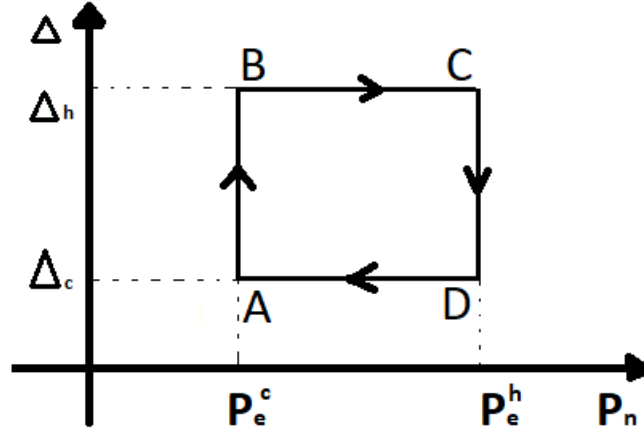


Figure 3.6: Quantum Otto cycle for a two-level system represented in $\Delta - P_n$ diagram, where Δ is the energy gap and P_n is the occupation probability.

processes. Since we will use this cycle in chapter 4, we will give a more detailed analysis of this kind of engine compared to the Carnot engine described previously.

Let's consider a generic quantum substance ruled by some Hamiltonian $\mathcal{H}(\lambda)$, where λ is an external parameter that is controllable by the experimenter, in contact with two heat baths. Then we get three parameters: λ , $\beta_h = 1/k_B T_h$ and $\beta_c = 1/k_B T_c$. The four-strokes of the Otto cycle are the following:

- **Adiabatic compression:** This is the first stroke of the Otto engine where the system begins thermalized with a cold heat bath at inverse temperature β_c and in the equilibrium Gibbs thermal state, $\rho(\lambda_i) = e^{-\beta_c \mathcal{H}(\lambda_i)} / Z(\lambda_i)$, where λ_i , $E_n(\lambda_i)$ and $Z(\lambda_i) = \text{Tr}[e^{-\beta_c \mathcal{H}(\lambda_i)}]$ are the initial value of the external parameter, the n^{th} eigenvalue of the system's Hamiltonian and the canonical partition function. In this process we detach the working substance from the cold bath and make an adiabatic change in the external parameter from its initial value to a final one, $\lambda_i \rightarrow \lambda_f$, which may change the eigenstates besides the eigenvalues. If the process takes enough time, according to the quantum adiabatic condition, it ensures that there won't be a change in the occupation probabilities ($dP_n = 0$). We also assume that there is no energy levels crossing while λ is changed. In this sense, the only energy contribution during this stroke is in form of work. This process is analogous to an adiabatic compression of an ideal gas. The work done here is given by

$$W_I = \sum_n \int_A^B P_n dE_n = \sum_n P_n^c(A) [E_n(B) - E_n(A)], \quad (3.2.2.1)$$

where $P_n^c = e^{-\beta_c E_n} / Z(\lambda)$ is the occupation probability of the n^{th} energy level of the system in thermal equilibrium with the cold bath and $P_n^c(A) = P_n^c(B)$.

- **Isochoric (hot):** In this second step, we connect the working substance with a hot heat bath at inverse temperature β_h with a fixed external parameter λ_f until it reaches the equilibrium Gibbs thermal state, $\rho(\lambda_f) = e^{-\beta_h \mathcal{H}(\lambda_f)} / Z(\lambda_f)$. During this thermalization stroke the system receives energy from the heat reservoir given by

$$\langle Q_h \rangle = \sum_n \int_B^C E_n dP_n = \sum_n E_n(B) [P_n^h(C) - P_n^c(A)], \quad (3.2.2.2)$$

where $P_n^h = e^{-\beta_h E_n} / Z(\lambda)$ is the occupation probability of the n^{th} energy level of the system in thermal equilibrium with the hot bath. No work is done and only heat is exchanged during this step.

- **Adiabatic expansion:** This third stroke is basically the inverse of the first one. We bring back the external parameter from λ_f to its initial value λ_i , while the occupation probabilities remain the same, P_n^h . Only work is done during this step and is given by

$$W_{II} = \sum_n \int_C^D P_n dE_n = \sum_n P_n^h(C) [E_n(A) - E_n(B)], \quad (3.2.2.3)$$

where $P_n^h(C) = P_n^h(D)$ and $E_n(A) = E_n(D)$, $E_n(B) = E_n(C)$.

- **Isochoric (cold):** This last step consists of putting the working substance in contact with a cold heat bath at inverse temperature β_c until it reaches the equilibrium state once again, $\rho(\lambda_i) = e^{-\beta_c \mathcal{H}(\lambda_i)} / Z(\lambda_i)$. No work is done in this process, only heat is released by the system into the cold bath. From the definition of heat in quantum mechanics, eq.(2.3.1.11), one can calculate the exchanged heat during this stroke as:

$$\langle Q_c \rangle = \sum_n \int_D^A E_n dP_n = \sum_n E_n(A) [P_n^c(A) - P_n^h(C)]. \quad (3.2.2.4)$$

Due to the energy conservation law, eq.(2.3.1.5), the net work done in a complete cycle is equal to the negative heat exchanged during both isochoric strokes in steps 2 and 4. For the rest of this dissertation we will use the convention that the net work done by the system is negative. From the equation of the heat exchange presented above for the Otto cycle, one can calculate the net work as:

$$\begin{aligned} W &= -(\langle Q_h \rangle + \langle Q_c \rangle) \\ &= -\sum_n \Delta E_n \Delta P_n, \end{aligned} \quad (3.2.2.5)$$

where $\Delta E_n = E_n(B) - E_n(A)$, $\Delta P_n = P_n(C) - P_n(A)$ and $W < 0$ indicates the work performed by the system. Then, the efficiency of the quantum Otto engine is given by

$$\begin{aligned} \eta &= -\frac{W}{\langle Q_h \rangle} \\ &= 1 - \frac{\sum_n E_n(A)}{\sum_n E_n(B)}. \end{aligned} \quad (3.2.2.6)$$

Where the condition $\sum_n E_n(A) > \sum_n E_n(B)$ must be fulfilled for the system to work as a heat engine. Implementations of Otto engines and other quantum engines and refrigerators can be found in the references [109, 118, 122, 123, 124, 125].

Two-level quantum Otto cycle

Let's give an example of a quantum Otto cycle for a simple two-level system [10]. This system has two energy levels given by E_g and E_e corresponding to the ground and excited eigenstates

$|\psi_g\rangle$ and $|\psi_e\rangle$, respectively, and an energy gap Δ between them. The Hamiltonian and the density matrix of this system in thermal equilibrium at temperature T are given by

$$\mathcal{H} = (E_e - E_g) |\psi_e\rangle\langle\psi_e|, \quad (3.2.2.7)$$

$$\rho^{eq} = P_g |\psi_g\rangle\langle\psi_g| + P_e |\psi_e\rangle\langle\psi_e|, \quad (3.2.2.8)$$

where P_g and P_e are the occupation probabilities of the ground and excited states. Let's consider the four strokes protocol presented above. Note that, as seen in eq.(3.1.0.2), in this case an effective temperature may be defined at all points along the cycle.

The system begins in thermal equilibrium at the inverse temperature β_c at the point A . The first stroke is the adiabatic compression. During this process no heat is exchanged and only work is done by changing the controllable external parameter, which takes the energy gap from Δ_i to a new one Δ_f , without changing the population ($P_{g(e)}(A) = P_{g(e)}(B)$). The work done in this stroke is given by eq.(3.2.2.1):

$$\begin{aligned} W_{A \rightarrow B}^I &= [E_e(B) - E_g(B)]P_e(B) - [E_e(A) - E_g(A)]P_e(B) \\ &= (\Delta_f - \Delta_i)P_e(B), \end{aligned} \quad (3.2.2.9)$$

where $\Delta_i = E_e(A) - E_g(A)$ and $\Delta_f = E_e(B) - E_g(B)$ and we use the fact that $P_g = 1 - P_e$.

The second stroke is the isochoric branch, during which the working substance is connected with a hot heat bath at the inverse temperature β_h at the point C . Before the system reaches this temperature, it can be described by the effective temperature $T_B^{eff} = (\Delta_f/\Delta_i)T_A$ at the point B . The exchanged heat released into the system, which is done without changing the energy and only varying the population, is given by eq.(3.2.2.2):

$$\begin{aligned} \langle Q^h \rangle_{B \rightarrow C} &= [E_e(C) - E_g(C)]P_e(C) - [E_e(B) - E_g(B)]P_e(B) \\ &= \Delta_f(P_e(C) - P_e(B)), \end{aligned} \quad (3.2.2.10)$$

where we use the fact that $E_g(B) = E_g(C)$ and $E_e(B) = E_e(C)$ and $\Delta_f = E_e(B) - E_g(B)$

The third stroke is the second adiabatic process where a compression is made in order to bring back the energy gap from Δ_f to Δ_i . Just like the adiabatic expansion, only work is done in this process while no heat is exchanged. And just like before, at the point D : $T_D^{eff} = (\Delta_i/\Delta_f)T_C$ and $P_{g(e)}(C) = P_{g(e)}(D)$. The work done is given by eq.(3.2.2.3):

$$\begin{aligned} W_{C \rightarrow D}^{II} &= [E_e(D) - E_g(D)]P_e(D) - [E_e(C) - E_g(C)]P_e(D) \\ &= (\Delta_i - \Delta_f)P_e(D). \end{aligned} \quad (3.2.2.11)$$

The last stroke is the final thermalization with the cold heat bath at inverse temperature β_c , where the system recovers its initial state and we use the fact that $E_g(A) = E_g(D)$ and $E_e(A) = E_e(D)$. From eq.(3.2.2.4):

$$\begin{aligned} \langle Q^c \rangle_{D \rightarrow A} &= [E_e(A) - E_g(A)]P_e(A) - [E_e(D) - E_g(D)]P_e(D) \\ &= \Delta_i(P_e(A) - P_e(D)), \end{aligned} \quad (3.2.2.12)$$

The efficiency of the two-level Otto cycle is given by eq.(3.2.2.6) together with the above equations just presented and the conditions, $P(A) = P(B)$ and $P(C) = P(D)$, and leads to:

$$\begin{aligned}\eta &= -\frac{(W_I + W_{II})}{\langle Q^h \rangle_{B \rightarrow C}} \\ &= \frac{(\Delta_f - \Delta_i)(P(A) - P(D))}{\Delta_f(P(A) - P(D))} \\ &= 1 - \frac{\Delta_i}{\Delta_f}.\end{aligned}\tag{3.2.2.13}$$

Just as expected from eq.(3.2.2.6) for a two-level system in a Otto cycle in quantum regime.

3.3 Measurement-based Otto cycle

In the previous section we showed the basic quantum version of two of the most important heat engines studied by the community of quantum thermodynamics, the Carnot and Otto cycles. Other kinds of cycles were already studied in their quantum version, such as Brayton cycle and Diesel cycle [36, 126, 127, 128, 129, 130, 131, 132, 133]. Several different setups for engines were already proposed in order to explore the relevance of quantum features in such thermal machines, trying to understand if any one of them could help boost the power and efficiency [134, 135]. Some of these approaches includes different types of baths coupled to the system beyond thermal baths, such as coherently-superposed bath [136, 137, 138], superradiant atomic systems [139], squeezed baths [140], strong system-bath coupling [135, 141, 142]. Besides these approaches, there is a new one that has began to be explored only in the last few years, the quantum measurement-based engines.

The idea of using a measurement first emerged as an application of the Maxwell's demon. As explained in section (2.5), the demon uses information about the system to extract work from it, work that could not be extracted before without the knowledge of the information acquired. Some of these works can be found in the references [143, 144, 145, 146, 147, 148, 149]. Such protocols are also known as feedback control protocols.

In this section we will present a new kind of heat engine proposed in 2017, by Juyeon Yi, Peter Talkner et. al. [55]. In their work, the quantum measurement approach is used in a different way compared to the other proposals presented in the literature so far. Previously, the measurement was being used to extract information about the system, and its outcome was used to decide the next step to be performed in order to extract work from the engine. In contrast, the measurement in Talkner's engine is meant to be used as a replacement for the hot heat bath, injecting heat into the system. In this sense, we can say that this new kind of measurement-based engine does not need a feedback control, unlike the Maxwell's demon based engines proposals. In their original work, they gave only two simple examples with single-particle systems. Later, in 2018, they studied such measurement-based engine with details in a more realistic scenario, using a harmonic oscillator as working substance, providing the engine's setup with a non-perfect thermalization stroke, different speeds of the work strokes and different strengths of energy injected by the measurement [150].

3.3.1 Single-bath Otto cycle without feedback control

Let's consider the quantum Otto cycle once again, but this time we will change the original setup by replacing the hot heat bath by a quantum measurement instead.

The system under consideration is a generic quantum system given by the density matrix

$$\rho(\lambda) = \sum_n P_n^{eq}(\lambda) |n, \lambda\rangle \langle n, \lambda|, \quad (3.3.1.1)$$

where P_n^{eq} is the occupation probability at thermal equilibrium. The system is ruled by the Hamiltonian

$$\mathcal{H}(\lambda) = \sum_n E_n(\lambda) |n, \lambda\rangle \langle n, \lambda|, \quad (3.3.1.2)$$

where λ is the external parameter, controllable by the experimenter. The energies $E_n(\lambda)$ are assumed to be non-degenerated for all possible values of λ . Note that we are considering the general case where the eigenvectors that may depend on some parameter, unlike we did in the chapter 2. Let us follow the four-strokes sequence presented in section (3.2.2). The system starts initially in thermal equilibrium with the only heat bath at inverse temperature β , which we consider as the cold heat bath since the measurement will replace the hot heat bath, and the initial value of the external parameter λ_i .

The work is done in the first adiabatic stroke by changing the external parameter, $\lambda_i \rightarrow \lambda_f$, and is given by eq.(3.2.2.1):

$$\langle W_I \rangle = \sum_n [E_n(\lambda_f) - E_n(\lambda_i)] P_n^{eq}(\lambda_i), \quad (3.3.1.3)$$

where $P_n^{eq}(\lambda_i) = e^{-\beta \mathcal{H}(\lambda_i)} / Z$ is the occupation probability of the system in thermal equilibrium with the single-bath. At the end of this process, the system is described by the density matrix $\rho_I(\lambda_f) = \sum_n P_n^{eq} |n, \lambda_f\rangle \langle n, \lambda_f|$. Note that the population does not change, as it should be the case for an adiabatic process, but the eigenvalues and eigenstates may change.

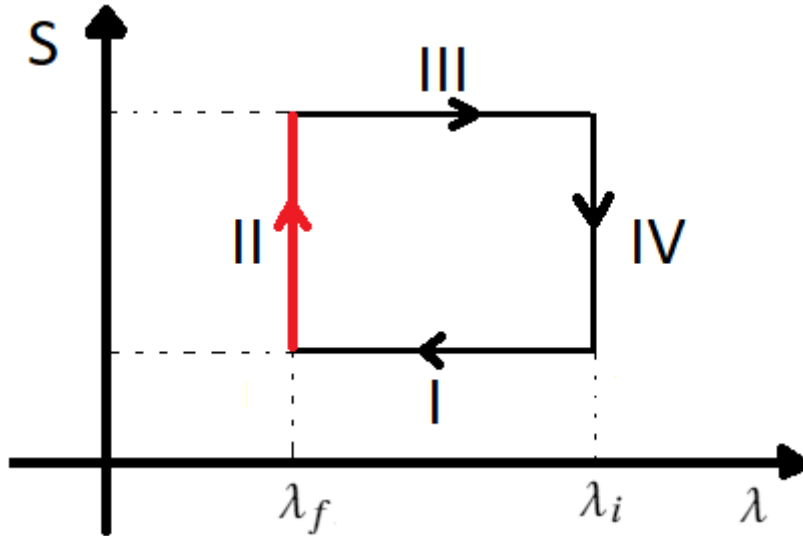


Figure 3.7: Measurement quantum Otto cycle without feedback control for any system which is controlled by an external parameter. Steps I and III are the adiabatic strokes, step II is the quantum measurement that replaces the hot heat bath and IV is the thermalization stroke.

The second stroke consists in a quantum measurement. Consider a measurement given by any general trace-preserving measure given by the Kraus operators, i.e., operators M_α that obey the relation $\sum_\alpha M_\alpha^\dagger M_\alpha = 1$. If the measurement operators commutates with the Hamiltonian, $[M_\alpha, \mathcal{H}] = 0$, then the system won't be disturbed. Therefore, the energy won't change. For example, consider a spin-1/2 system described by a density matrix ρ diagonal in the energy basis and ruled by the Hamiltonian

$$\mathcal{H} = \hbar w \sigma_z, \quad (3.3.1.4)$$

where σ_z is the Pauli matrix in the z-direction and w is the frequency. If we perform a measurement in the system with the operators $M_\pm = (1 \pm \sigma_z)/2$, corresponding to a projective measurement of σ_z , the density matrix after a non-selective measurement will be given by $\rho' = \sum_i M_i \rho M_i^\dagger$. For the chosen measurement operators M_\pm , we get $\rho' = M_+ \rho M_+^\dagger M_- \rho M_-^\dagger = \rho$. It is clear that the system was not disturbed by this measurement, since the initial and final density matrix are the same. Thus, the energy difference before and after the measurement is be given by: $\Delta U = \text{Tr}[\mathcal{H} \rho'] - \text{Tr}[\mathcal{H} \rho] = \text{Tr}[\mathcal{H}(\rho' - \rho)] = 0$, since $\rho' = \rho$. In this sense, since the system is not disturbed, it's energy does not change. Later we shall give an example where the measurement disturbs the system when we choose M_α operators corresponding to spin measurements along a different axis.

If the operators do not commute, the system will be disturbed in such way that its energy will be changed. The final state of the system after the measurement is given by

$$\rho^{PM} = \sum_\alpha M_\alpha \rho_I(\lambda_f) M_\alpha^\dagger. \quad (3.3.1.5)$$

The averaging over all possible states, i.e., non-selective measurement, means that there is no feedback mechanism. It can be seen as a quantum channel that takes one density matrix into a new one, without acquiring any information during the process. The population after this process won't be given by the thermal state as before. It will be given by

$$\begin{aligned} P_n^{PM} &= \langle n, \lambda_f | \rho^{PM} | n, \lambda_f \rangle = \langle n, \lambda_f | \sum_\alpha M_\alpha \rho_I(\lambda_f) M_\alpha^\dagger | n, \lambda_f \rangle \\ &= \sum_m P_m^{eq}(\lambda_i) \sum_\alpha \langle n, \lambda_f | M_\alpha | m, \lambda_f \rangle \langle m, \lambda_f | M_\alpha^\dagger | n, \lambda_f \rangle \\ &= \sum_m T_{m,n} P_n^{eq}(\lambda_i), \end{aligned} \quad (3.3.1.6)$$

where $T_{m,n} = \sum_\alpha \left| \langle m, \lambda_f | M_\alpha | n, \lambda_f \rangle \right|^2 > 0$ are the elements of a transfer matrix that satisfies the following condition: $\sum_m T_{m,n} = \sum_\alpha \langle n | M_\alpha^\dagger (\sum_m |m\rangle \langle m|) M_\alpha | n \rangle = \langle n | \sum_\alpha M_\alpha^\dagger M_\alpha | n \rangle = 1$. From the definition of $T_{m,n}$, we can interpret it as the conditional probability $p(m|n)$ that the system ends up in state $|m\rangle$ if it was initially in state $|n\rangle$. The energy exchanged during this process can be written as

$$\begin{aligned}
\langle Q_M \rangle &= \langle \mathcal{H}_M(\lambda_f) \rangle - \langle \mathcal{H}(\lambda_f) \rangle = \text{Tr}[\rho_I(\lambda_f)(\mathcal{H}_M(\lambda_f) - \mathcal{H}(\lambda_f))] \\
&= \sum_n E_m(\lambda_f) [P_m^{PM} - P_m^{eq}(\lambda_i)] = \sum_m E_m(\lambda_f) \langle m, \lambda_f | \rho^{PM} - \rho_I(\lambda_f) | m, \lambda_f \rangle \\
&= \sum_{n,m} \langle m, \lambda_f | \left(\sum_\alpha (M_\alpha |n, \lambda_f\rangle \langle n, \lambda_f| M_\alpha^\dagger) - |n, \lambda_f\rangle \langle n, \lambda_f| \right) P_n^{eq}(\lambda_i) | m, \lambda_f \rangle E_m(\lambda_f) \\
&= \sum_{n,m} \left[T_{m,n} P_n^{eq}(\lambda_i) E_m(\lambda_f) - \delta_{n,m} P_n^{eq}(\lambda_i) E_m(\lambda_f) \right] \\
&= \sum_{n,m} \left[T_{m,n} E_m(\lambda_f) - \delta_{n,m} E_n(\lambda_f) \right] P_n^{eq}(\lambda_i),
\end{aligned} \tag{3.3.1.7}$$

where $\mathcal{H}_M(\lambda_f) = \sum_\alpha M_\alpha^\dagger \mathcal{H}(\lambda_f) M_\alpha$. Note that we do not assume any property on the operators M_α so far. In principle the quantity $\langle Q_M \rangle$ can be either positive or negative. This energy exchange generated by the measurement process can be interpreted as a contact of the system with a non-thermal bath.

We can rewrite eq.(3.3.1.7) by using the relation $\sum_{n,m} \delta_{n,m} P_n^{eq}(\lambda_i) E_n(\lambda) = \sum_{n,m} T_{n,m} P_n^{eq}(\lambda_i) E_n(\lambda)$ as

$$\begin{aligned}
\langle Q_M \rangle &= \sum_{n,m} (E_m(\lambda_f) - E_n(\lambda_f)) T_{m,n} P_n^{eq}(\lambda_i) \\
&= \sum_{n,m} T_{m,n} \Delta_{m,n}^f P_n^{eq}(\lambda_i),
\end{aligned} \tag{3.3.1.8}$$

where $\Delta_{m,n}^f = E_m(\lambda_f) - E_n(\lambda_f)$ and the term $T_{m,n} P_n^{eq}(\lambda_i)$ can be seen as the joint probability that the system begins in the state $|n\rangle$ and ends in state $|m\rangle$, gaining energy in the process.

Now, considering a subset of Unital measurement operators used by the authors in reference [55], namely minimal disturbance measurements (MDM), $M_\alpha = M_\alpha^{\dagger 1}$, the T matrix becomes symmetric:

$$T_{n,m} = \sum_\alpha \left| \langle n, \lambda_f | M_\alpha | m, \lambda_f \rangle \right|^2 = \left| \langle m, \lambda_f | M_\alpha^\dagger | n, \lambda_f \rangle \right|^2 = \left| \langle m, \lambda_f | M_\alpha | n, \lambda_f \rangle \right|^2 = T_{m,n}. \tag{3.3.1.9}$$

Using this result we can rewrite the measurement heat one more time to finally get

$$\langle Q_M \rangle = \frac{1}{2} \sum_{n,m} [E_m(\lambda_f) - E_n(\lambda_f)] T_{m,n} (P_n^{eq}(\lambda_i) - P_m^{eq}(\lambda_i)), \tag{3.3.1.10}$$

which is the final equation for the measurement heat presented by the authors in reference [55].

Since the system is initially in a thermal state, $\rho_I(\lambda_i)$, and we assume that there is no population inversion, it leads to the following occupation probability ordering: $P_n^{eq}(\lambda_i) > P_m^{eq}(\lambda_i) \iff E_n(\lambda_i) < E_m(\lambda_i)$. If there is no level crossing for all values of λ , then we have $E_n(\lambda_i) < E_m(\lambda_i) \iff E_n(\lambda_f) < E_m(\lambda_f)$ as well. Thus, since all terms in eq.(3.3.1.10) are positive, it implies the injection of energy $\langle Q_M \rangle \geq 0$. If there is some energy level crossing, the heat can be negative.

The third stroke is another adiabatic process that reverts the first stroke. By taking back the external parameter to its initial value, $\lambda_f \rightarrow \lambda_i$, the system is taken to a new state given by

¹This is a sufficient mathematical feature chosen by the authors that guarantees $\langle Q_M \rangle > 0$.

$$\rho^{PM} \rightarrow \rho_{III} = \sum_n P_n^{PM} |n, \lambda_i\rangle \langle n, \lambda_i|. \quad (3.3.1.11)$$

Then, the work done in this process is given by

$$\langle W_{II} \rangle = \sum_n [E_n(\lambda_i) - E_n(\lambda_f)] P_n^{PM}. \quad (3.3.1.12)$$

As before, if $E_n(\lambda_f) > E_n(\lambda_i)$, then $\langle W_{II} \rangle \leq 0$.

The last stroke is the only isochoric process in this protocol. The system is put in contact with the only heat bath until it thermalizes and reaches the thermal state once again, completing the cycle. The heat exchange in this stroke is given by

$$\begin{aligned} \langle Q_c \rangle &= \sum_n E_n(\lambda_i) [P_n^{eq}(\lambda_i) - P_n^{PM}] \\ &= \sum_{n,m} [\delta_{m,n} E_n(\lambda_i) - T_{m,n} E_n(\lambda_i)] P_m^{eq}. \end{aligned} \quad (3.3.1.13)$$

Comparing with the measurement heat equation, eq.(3.3.1.7), we can apply the same considerations as before and rewrite equation above as

$$\begin{aligned} \langle Q_c \rangle &= \frac{1}{2} \left[\sum_{n,m} T_{m,n} (E_m(\lambda_i) - E_n(\lambda_i)) P_m^{eq}(\lambda_i) + \sum_{n,m} T_{n,m} (E_n(\lambda_i) - E_m(\lambda_i)) P_n^{eq}(\lambda_i) \right] \\ &= \frac{1}{2} \sum_{m,n} (E_m(\lambda_i) - E_n(\lambda_i)) \left[T_{m,n} P_m^{eq}(\lambda_i) - T_{n,m} P_n^{eq}(\lambda_i) \right]. \end{aligned} \quad (3.3.1.14)$$

Since the transfer matrix is symmetric, $T_{n,m} = T_{m,n}$, we get the final expression:

$$\langle Q_c \rangle = \frac{1}{2} \sum_{m,n} \left[\Delta_{m,n}^i T_{m,n} (P_m^{eq}(\lambda_i) - P_n^{eq}(\lambda_i)) \right], \quad (3.3.1.15)$$

where $\Delta_{m,n}^i = E_m(\lambda_i) - E_n(\lambda_i)$. As we saw before, if the condition $E_m(\lambda_i) > E_n(\lambda_i) \iff P_m^{eq}(\lambda_i) < P_n^{eq}(\lambda_i)$ holds for thermal states, then we ensure that the heat flux is in the direction from the system to the heat bath, using it as a sink, $\langle Q_c \rangle < 0$.

Energy conservation and efficiency

Let's consider now the energy conservation as stated in eq.(2.3.1.11). The total heat exchange, injected into the system by the measurement and released from the system to the heat bath during the thermalization, is given by

$$\begin{aligned} \langle Q_M \rangle + \langle Q_c \rangle &= \sum_{m,n} T_{m,n} [\Delta_{m,n}^f P_n^{eq}(\lambda_i) + \Delta_{m,n}^i P_m^{eq}(\lambda_i)] \\ &= \sum_{m,n} T_{m,n} \Delta_{m,n}^f P_n^{eq}(\lambda_i) + T_{n,m} \Delta_{n,m}^i P_n^{eq}(\lambda_i) \\ &= \sum_n \left(\sum_m [T_{m,n} \Delta_{m,n}^f - T_{m,n} \Delta_{m,n}^i] P_n^{eq}(\lambda_i) \right) \\ &= \sum_{m,n} T_{m,n} (\Delta_{m,n}^f - \Delta_{m,n}^i) P_n^{eq}(\lambda_i), \end{aligned} \quad (3.3.1.16)$$

where we use the fact that $T_{m,n}$ is symmetric and $\Delta_{m,n}^f = E_m(\lambda_f) - E_n(\lambda_f)$. Considering the energy conservation, the total work must be equal to the negative value of the total heat exchange. So we must get

$$\begin{aligned}
\langle W_T \rangle &= \langle W_I \rangle + \langle W_{II} \rangle \\
&= -(\langle Q_M \rangle + \langle Q_C \rangle) \\
&= \sum_n \left(\sum_m T_{n,m} \Delta_{m,n}^i - T_{m,n} \Delta_{m,n}^f \right) P_n^{eq}(\lambda_i) \\
&= \frac{1}{2} \sum_{n,m} (\Delta_{m,n}^f - \Delta_{m,n}^i) T_{m,n} (P_m^{eq}(\lambda_i) - P_n^{eq}(\lambda_i)).
\end{aligned} \tag{3.3.1.17}$$

To determine the sign of the net work, we must consider the sign of $\Delta_{m,n}^{i(f)}$. Let's first consider the case where $\Delta_{m,n}^i > 0$: The energy gap between the levels grows in the adiabatic compression process while the external parameter changes from λ_i to λ_f , leading to $\Delta_{m,n}^f > \Delta_{m,n}^i$. Since the canonical probability distribution $P_n^{eq}(\lambda_i)$ decreases monotonically with the increase of the energy $E_n(\lambda_i)$, the difference between two levels n and m will be negative, $P_m^{eq}(\lambda_i) - P_n^{eq}(\lambda_i) < 0$. Similarly, for $\Delta_{m,n}^i < 0$, all considerations taken before are still valid, so $\Delta_{m,n}^f \leq \Delta_{m,n}^i$, leading to $P_m^{eq}(\lambda_i) - P_n^{eq}(\lambda_i) \geq 0$. For both cases the elements of the transfer matrix are always positive, $T_{m,n} \geq 0$. Taking all of this into account, the contribution of the net work is always negative.

Finally, we can calculate the efficiency of the measurement-based quantum Otto engine. Taking the equations (3.3.1.17), (3.3.1.10) into (3.2.2.6), one gets

$$\begin{aligned}
\eta &= -\frac{\langle W_T \rangle}{\langle Q_M \rangle} \\
&= 1 - \frac{\sum_{n,m} T_{m,n} \Delta_{m,n}^i P_n^{eq}(\lambda_i)}{\sum_{n,m} T_{m,n} \Delta_{m,n}^f P_n^{eq}(\lambda_i)}.
\end{aligned} \tag{3.3.1.18}$$

This efficiency is always smaller than 1, in total agreement with the second law.

Qubit example

For a simple example, we will present the spin-1/2 system as working substance, just like the one present in Yi and Talkner's paper [55]. Let's consider that this spin-1/2 is in the presence of an external magnetic field in z -direction, which is our external parameter $\lambda = B_z$. The Hamiltonian is given by

$$\mathcal{H}(B) = -\mu_B B \sigma_z, \tag{3.3.1.19}$$

where μ_B is the Bohr magneton and σ_z is the Pauli spin matrix in z direction. The Hamiltonian's eigenvalues are given by $E_{\pm} = \mp \mu_B B$, where the positive (negative) sign indicates the two possible eigenstates of the system: spin up and spin down, respectively. The system is initially in thermal state at inverse temperature $\beta_c = 1/k_B T_c$, represented by the density matrix $\rho(B_0) = e^{-\beta_c \mathcal{H}(B_0)} / Z$, with $Z = 2 \cosh(\beta_c \mu_B B_0)$ and the occupation probability of both states is specified by $P_{\pm}^{eq} = e^{\pm \beta_c \mu_B B_0} / Z$.

The work done in the first stroke, the adiabatic compression process, is given by

$$\langle W_I \rangle = \mu_B (B_0 - B_1) \tanh(\beta_c \mu_B B_0) < 0, \quad (3.3.1.20)$$

where the magnetic field was increased from B_0 to $B_1 > B_0$.

The general measurement operator of this engine is given by a projective measurement in x -direction bases of Pauli matrix:

$$M_{\pm} = \frac{(1 \pm \sigma_x)}{2}, \quad (3.3.1.21)$$

which yields to the transition probability $T_{\pm, \pm} = 1/2$ between all combinations of possible state transitions. The final occupation probability after the measurement is uniform for both levels, $P_{\pm}^{PM} = 1/2$. The energy injected by this specific measurement during this stroke can be written as

$$\langle Q_M \rangle = \mu_B B_1 \tanh(\beta_c \mu_B B_0) > 0. \quad (3.3.1.22)$$

The work done in the adiabatic expansion is zero, due to the uniform population after the measurement. So the net work done in the cycle is done only during the adiabatic compression, $\langle W_T \rangle = \langle W_I \rangle$. The last energy exchange is made in the final stroke, where the system releases energy into the cold heat bath, and it is given by eq.(3.3.1.15):

$$\langle Q_c \rangle = -\mu_B B_0 \tanh(\beta_c \mu_B B_0). \quad (3.3.1.23)$$

Finally, putting all these equations together, we can calculate the efficiency as

$$\eta_0 = 1 - \frac{B_0}{B_1}. \quad (3.3.1.24)$$

This efficiency will be used in next chapter as a limit to the Otto cycle which we will wish to surpass.

Part II

Results

Three-level system as working substance

In chapter 2 we briefly reviewed some important fundamental concepts of classical thermodynamics like work, heat, pressure, the four basic thermodynamics processes and studied their extension to the quantum theory regime. In chapter 3 we applied all these concepts to two of the most important thermodynamic cycles, Carnot and Otto cycles. There we showed that the efficiency of these quantum heat engines is the same as their classical counterpart. Besides, the Carnot efficiency is still the upper bound to any heat engine's efficiency both in classical and quantum cases, working between two thermal heat baths at temperatures T_c and T_h [151].

In reference [117], the author studied the same Otto quantum cycle, presented in section (3.2.2) of chapter 3, for a two coupled qubit system interacting via Heisenberg Hamiltonian. There, the engine's efficiency was shown to be higher when the interaction between both qubits is non-zero. The mechanism behind this phenomenon was explained in terms of local heat energy exchanged. Local heat energy is defined as an energy that is separately exchanged between each subsystem with the thermal heat bath. This definition becomes confusing when there is some interaction between the subsystems.

In the last section of chapter 3, we also described the proposal of a new thermal engine, first presented by Talkner et al. in 2017 [55]. This new proposal works with a single-bath setup, which is used as a heat sink to the energy dumped by the working substance, and applies a quantum measurement as an energy source. This measurement process must satisfy some constraints in order to ensure the energy injection. After this work, they studied the same single-bath measurement-based heat engine in a more realistic scenario, where they used a quantum harmonic oscillator as working substance, considering a perfect and imperfect thermalization, different speeds of strokes and temperatures [150]. Later, a study was done with two coupled qubits interacting via a one dimension Heisenberg Hamiltonian [152]¹. It was shown that the coupling between both qubits can boost the efficiency somehow, depending on the directions chosen to realize the projective spin measurement. However, it was not clear how the interaction boosts the efficiency beyond the uncoupled case, where the engine works with two separated qubits. The authors of [152] didn't use the local heat argument unlike what had been done previously for the same system in the two-bath model [117].

In this chapter, we will revisit both two-baths and measurement-based quantum Otto cycle models in order to study the mechanism responsible for the enhancement of the efficiency. For this purpose, we start our analysis with a simple toy model, which will be a simple three-level quantum system, e.g., a qutrit. With this simple model, we are able to explain the boost in the

¹The same system used in reference [117].

efficiency without invoking any quantum property, such as quantum correlations. Next, we extend this mechanism for the same Heisenberg Hamiltonian used in references [117, 152]. It becomes clear that the mechanism is valid for two interacting systems in the same way it works for the single qutrit system. In this sense, there is no need to invoke entanglement or any other quantum property to explain this efficiency enhancement for both types of engines.

4.1 Qutrit system as a QHE

In this section we will consider both the two-bath model, presented in section (3.2.2), and single-bath measurement-based quantum Otto heat engine, presented in section (3.3.1), consisting of a three-level quantum system, e.g., qutrit, as the working substance. As mentioned before, in principle, this is just a toy model that will help to understand the behavior of the efficiency for the Heisenberg model with two spins. The qutrit is ruled by the Hamiltonian

$$\mathcal{H}(B) = \begin{bmatrix} 0 & B & 0 \\ B & 0 & 0 \\ 0 & 0 & -J \end{bmatrix}, \quad (4.1.0.1)$$

where B is the external parameter and $-J$ is a fixed energy level, where $|B| > |J|$.

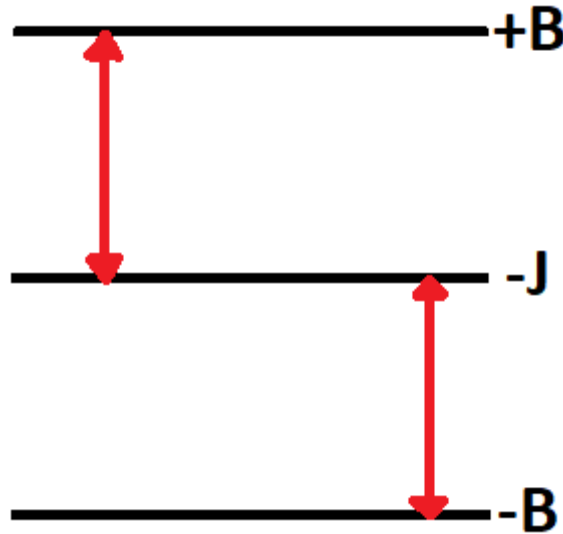


Figure 4.1: Three-level quantum system with two of them being dependent of the external parameter.

The Hamiltonian's eigenvalues are given in table (4.1) with their respective eigenvectors, where:

$$|0\rangle := \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, |1\rangle := \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, |2\rangle := \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \quad (4.1.0.2)$$

Eigenvalues	Eigenstates
$+B$	$(0\rangle + 1\rangle)/\sqrt{2}$
$-J$	$ 2\rangle$
$-B$	$(1\rangle - 0\rangle)/\sqrt{2}$

Table 4.1: The three eigenvalues of the Hamiltonian $\mathcal{H}(B)$ with their associated eigenvectors.

Note that the eigenvectors of this system do not depend on any parameter, just as we assumed previously in chapter 2 in eq.(2.3.1.9). So the Alicki's definitions of work and heat will be more appropriated as mentioned before.

In the next two sections, we will first study the efficiency of the quantum Otto engine with two baths and then study the measurement-based heat engine. In order to do so, we must analyse the work and heat produced in the process. From eq. (2.3.1.11) we can write the generic expressions for the exchanged heat for both models as

$$\langle Q_c \rangle = -B_i(\Delta P_B) + B_i(\Delta P_{-B}) + J(\Delta P_{-J}), \quad (4.1.0.3)$$

$$\langle Q_{h(M)} \rangle = B_f(\Delta P_B) - B_f(\Delta P_{-B}) - J(\Delta P_{-J}), \quad (4.1.0.4)$$

where $B_i < B_f$ are the initial and final value of this energy level, $\langle Q_h \rangle$ and $\langle Q_M \rangle$ are the heat absorbed by the system during the hot bath thermalization and by the measurement process, respectively, and $\Delta P_n = P_n^h - P_n^c$ is the population difference in the two-bath model. For the measurement-based model, this population difference is given by $\Delta P_n = P_n^{PM} - P_n^c$, where $P_n^{PM} = \sum_m T_{m,n} P_n^{eq}(\lambda_i)$ is dependent on the measurement. The total work is given by

$$\begin{aligned} \langle W \rangle &= -(\langle Q_c \rangle + \langle Q_{h(M)} \rangle) \\ &= -(B_f - B_i)(\Delta P_B - \Delta P_{-B}). \end{aligned} \quad (4.1.0.5)$$

We first should note that the work does not depend on the $-J$ energy level since this will be crucial to understanding the increase in the efficiency.

Looking at the eq.(4.1.0.3) and eq.(4.1.0.4), we note that it is possible to divide them into three parts. Each one of these parts can be separately associated with one of the energy levels. Since $\langle Q_c \rangle$ and $\langle Q_{h(M)} \rangle$ are the total energy flowing out and into the total system, we can interpret each separated part as an energy exchanged through each energy level. This interpretation, along with the fact that the $-J$ level does not contribute to the work, will be essential to explain the increase in the efficiency. Finally, defining the three separated terms as a function of the eigenvalues and the probabilities difference, $q_n = E_n(\Delta P_n)$, we can write the energy exchanged into each energy level during the first isochoric stroke (thermalization with the hot heat bath) as:

$$q_B = +B_f(\Delta P_B), \quad (4.1.0.6)$$

$$q_{-J} = -J(\Delta P_{-J}), \quad (4.1.0.7)$$

$$q_{-B} = -B_f(\Delta P_{-B}). \quad (4.1.0.8)$$

This expression and its interpretations are valid for both engine types. The only difference is the origin of the change in the population. While in the two bath model it came from a thermalization process, P_n^h , in the measurement model it depends on the measurement made, P_n^{PM} . The exchanged energy through each level for the second isochoric stroke is given by replacing $B_f \rightarrow B_i$ and $\Delta P_n \rightarrow -\Delta P_n$.

As it was done in reference [117], we can write the ratio of the quantum Otto engine for the qutrit and the qubit system in order to find a condition for the increase in the efficiency:

$$\begin{aligned} \frac{Q_{h(M)}}{Q_{h(M)}} = 1 &= \frac{-B_f(\Delta P_{-B} - \Delta P_{+B})}{Q_{h(M)}} - J \frac{\Delta P_{-J}}{Q_{h(M)}} \\ &= -\frac{B_f W}{(B_f - B_i)Q_{h(M)}} - J \frac{\Delta P_{-J}}{Q_{h(M)}} \\ &= \frac{\eta}{\eta_0} - J \frac{\Delta P_{-J}}{Q_{h(M)}}, \end{aligned} \quad (4.1.0.9)$$

where $\eta = -W/Q_{h(M)}$ and $\eta_0 = 1 - B_i/B_f$ are the qutrit efficiency and the qubit efficiency, respectively. Now we are able to rewrite this equation as a function of the energy exchanged through each energy level, q_n . So eq.(4.1.0.9) becomes:

$$\begin{aligned} \frac{\eta}{\eta_0} &= 1 + J \frac{\Delta P_{-J}}{Q_{h(M)}} \\ &= 1 - \frac{q_{-J}}{\langle Q_{h(M)} \rangle}. \end{aligned} \quad (4.1.0.10)$$

In reference [117], we believe that the author considered a misleading interpretation of the function q_n as a local heat exchange of each qubit of a two qubit system interacting via a Heisenberg Hamiltonian. This interpretation becomes confusing when the interaction between both qubits is strong enough to not be ignored. Here, we believe that by considering this function as the energy flow through each energy level, we can explain the mechanism behind the increase of the efficiency without this problem.

It is clear from eq.(4.1.0.10) that the term q_{-J} must be negative in order to observe an increase in the efficiency, since $\langle Q_{h(M)} \rangle = q_{-B} + q_{-J} + q_{+B} > 0^2$. In this sense, we can interpret this negative sign as an energy flowing in the opposite direction of the natural energy flux, as $\langle Q_{h(M)} \rangle > 0$, $q_{\pm B} > 0$ and $q_{-J} < 0$. Thus, as long as $q_{-J} < 0$, only the total energy $\langle Q_{h(M)} \rangle$ will decrease while the total work W will not change, since this energy level does not contribute to the work.

In sum, we just presented a new interpretation of a mechanism that can explain the boost in the efficiency for a quantum Otto heat engine with a three-level system. The crucial idea behind this mechanism leans on the energy level structure of the system, where at least one of the energy levels must not depend on the external parameter while the other ones must depend only on the external parameter in order to enhance the efficiency. In addition, this proposal is able to explain both the two-bath and measurement-based models of the Otto cycle's efficiency and no quantum properties, such as quantum correlations, are necessary for this mechanism to work.

²When there is no energy crossing.

4.1.1 Two-baths quantum Otto engine

The quantum Otto heat engine with two-baths setup begins with the qutrit in the equilibrium Gibbs thermal state thermalized with the cold heat bath at inverse temperature $\beta_c = 1/k_B T_c$. The population of each energy level in thermal equilibrium is given by

$$P_{+B} = \frac{e^{-\beta_c B_i}}{Z}, \quad (4.1.1.1)$$

$$P_{-J} = \frac{e^{\beta_c J}}{Z}, \quad (4.1.1.2)$$

$$P_{-B} = \frac{e^{\beta_c B_i}}{Z}, \quad (4.1.1.3)$$

where $Z = 2 \cosh(\beta_c B_i) + e^{\beta_c J}$ is the partition function and B_i is the initial value of the external parameter. The equilibrium state with the hot heat bath is given by replacing $\beta_c \rightarrow \beta_h$ and $B_i \rightarrow B_f$. From eq.(4.1.0.3) and eq.(4.1.0.4) we can calculate the heat exchanged in the two isochoric strokes, second and fourth steps of the Otto cycle. They are given by

$$\langle Q_h \rangle = \frac{-J e^{\beta_c J} + 2B_f \sinh(\beta_c B_i)}{2 \cosh(\beta_c B_i) + e^{\beta_c J}} - \frac{-J e^{\beta_h J} + 2B_f \sinh(\beta_h B_f)}{2 \cosh(\beta_h B_f) + e^{\beta_h J}}, \quad (4.1.1.4)$$

$$\langle Q_c \rangle = -\frac{-J e^{\beta_c J} + 2B_i \sinh(\beta_c B_i)}{2 \cosh(\beta_c B_i) + e^{\beta_c J}} + \frac{-J e^{\beta_h J} + 2B_i \sinh(\beta_h B_f)}{2 \cosh(\beta_h B_f) + e^{\beta_h J}}. \quad (4.1.1.5)$$

So we get the total work by the negative sum of both equations above:

$$\langle W \rangle = 2(B_i - B_f) \left(\frac{\sinh(\beta_c B_i)}{2 \cosh(\beta_c B_i) + e^{\beta_c J}} - \frac{\sinh(\beta_h B_f)}{2 \cosh(\beta_h B_f) + e^{\beta_h J}} \right). \quad (4.1.1.6)$$

Note that the positive work condition, $T_h > (B_f/B_i)T_c$, only holds when $J = 0$. Unfortunately, for the case where $J \neq 0$ there is no simple analytic expression for the negative work condition.

We are now able to calculate the efficiency from eq.(4.1.1.4) and eq.(4.1.1.6). It can be written as

$$\eta_T = \frac{(B_f - B_i)}{B_f + \Omega J}, \quad (4.1.1.7)$$

where

$$\Omega = \frac{e^{\beta_c(B_i+J)} + e^{\beta_c(B_i+J)+2\beta_h B_f} - e^{\beta_h(B_f+J)+2\beta_c B_i} - e^{\beta_h(B_f+J)}}{2(e^{2\beta_c B_i} - e^{2\beta_h B_f}) + e^{\beta_c(B_i+J)} - e^{\beta_h(B_f+J)} - e^{\beta_c(B_i+J)+2\beta_h B_f} + e^{\beta_h(B_f+J)+2\beta_c B_i}}. \quad (4.1.1.8)$$

Thereby, if the middle level $-J$ is equal to zero, we recover the qubit efficiency. According to the energy level structure of this specific system, the $\pm B$ levels becomes equidistant from the middle level 0. This is essentially the same as a qubit system.

From now on, we will set some values for our parameter: $B_i = 3$, $B_f = 4$, $\beta_h = 0.5$ and $\beta_c = 1$. These values will be used for the measurement-based engine as well, in order to compare both models in the fairest possible way.

In fig.(4.2) we show the total work (black curve), the heat exchange during the thermalization with the cold (blue curve) and hot bath (red curve). From this figure, it can be seen that the total work becomes zero at $J \approx 2.18$ for these set of chosen variables. For greater values of J the condition $W < 0$ does not hold anymore, thus the work becomes positive and we do not have a heat engine. For any change in the variables values, the cut limit of J will be different.

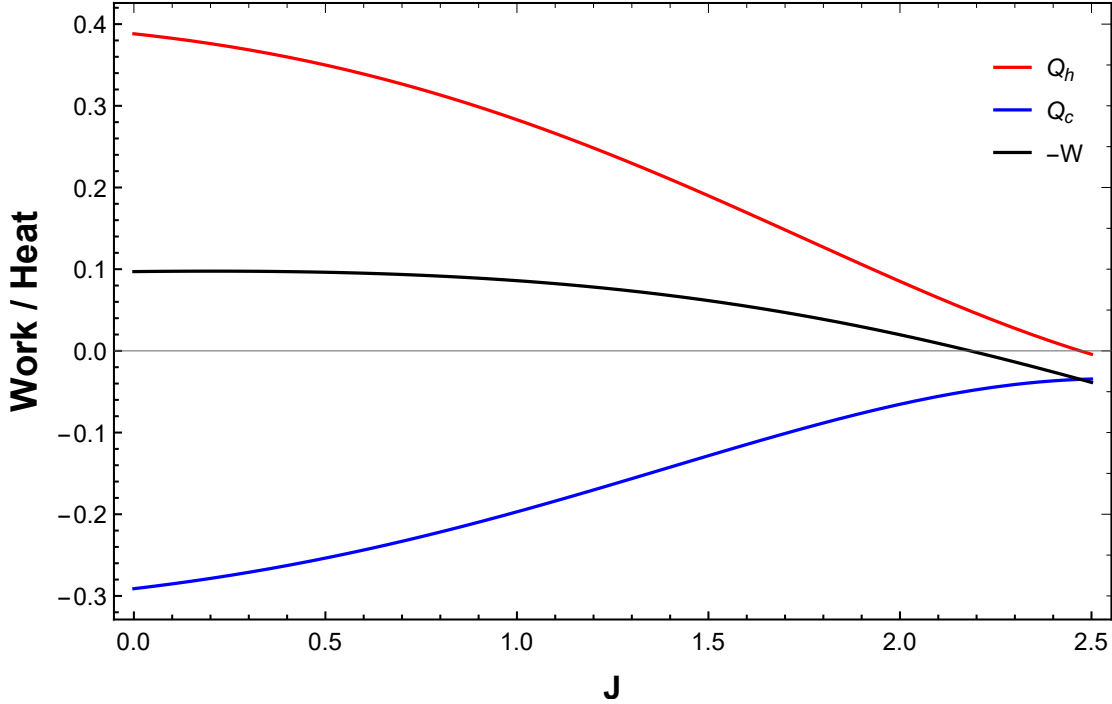


Figure 4.2: Total work and heat of a two-baths quantum Otto engine. Heat absorbed (red) by the system, heat released (blue) into the bath, total work (black) done on the system.

To illustrate our results, we plot in fig.(4.3) the efficiency as a function of J for fixed temperatures $T_h = 2$ and $T_c = 1$ and external parameters $B_i = 3$ and $B_f = 4$. At the zero value of J , the efficiency is the same as the qubit $\eta = \eta_0 = 1 - 3/4 = 0.25$. As this energy level becomes greater, the efficiency starts to increase until a certain value of J . From the inset figure, one can see the three energy exchanged in each one of the energy levels. As expected from eq.(4.1.0.10), the heat exchanged through the $-J$ energy level is negative from zero until the maximum value where the efficiency goes back to limit value, $\eta = 0.25$, around $J \approx 1.96$. For greater values of J , the efficiency becomes smaller than the qubit limit as q_{-J} becomes positive.

In sum, we showed that it is possible to increase the efficiency of a qutrit system. Therefore, it is not necessary to invoke any quantum properties, such as quantum correlations, to observe this effect. In fact, the energy levels structure of the system is enough to explain this increase in the efficiency: The one level that does not change with the external parameter and do not contribute to the work is an essential requirement. This level is responsible for the energy exchange in the opposite direction, due to the negative value of the function q_n associated with it, leading to a smaller value of Q_h without changing the work. We also gave a simple physical interpretation for the increase of the efficiency in terms of the energy exchanged through each energy level. However, the origin of this opposite energy exchanged is still not clear. It might come from the fact that the

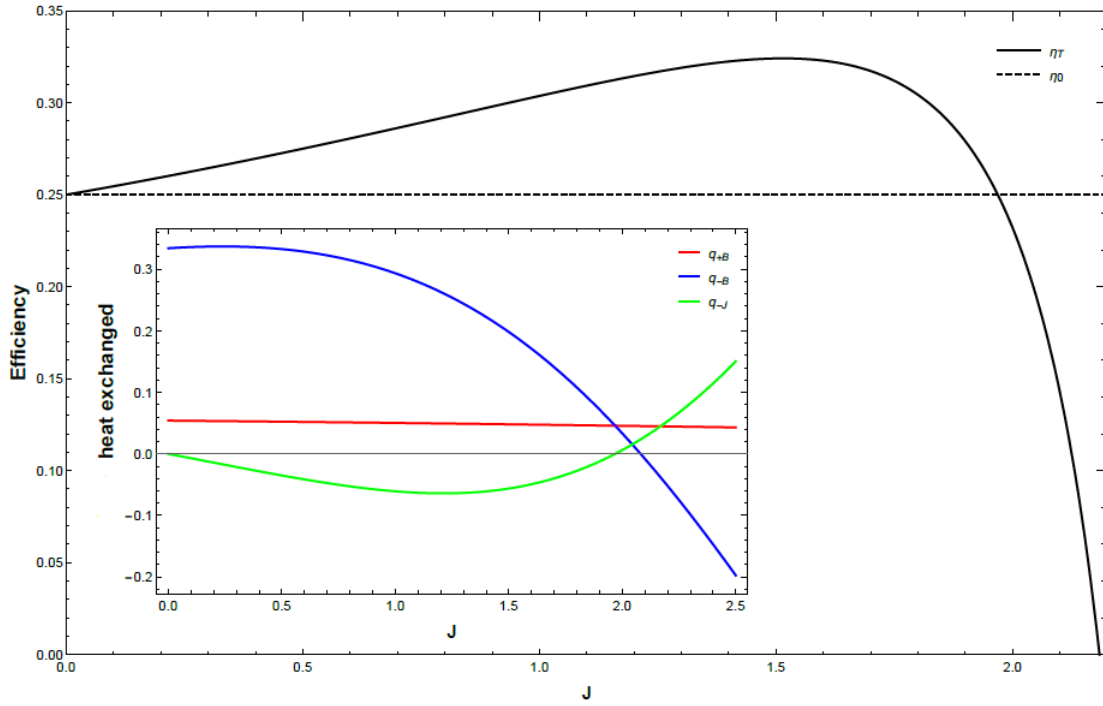


Figure 4.3: Efficiency of two baths quantum heat engine for a qutrit. (Dashed) η_0 is the efficiency for a two level limit case ($J \rightarrow 0$) and (Solid) η_T is the case with a third energy level ($-J$). (Inset) The heat flux through for each energy level. (Red) The exchanged heat in the $+B$ energy level. (Blue) The energy flux in the $-B$ energy level. (Green) The energy exchanged in the $-J$ level which is responsible for the increase of the efficiency.

system is in non-equilibrium states during the adiabatic or the measurement processes, but more investigation must be done in order to achieve a better understanding.

4.1.2 Measurement-based quantum Otto engine

Let's consider the second quantum heat engine protocol presented in chapter 3. Since the measurement stroke replaces the hot heat bath, the population after the measurement will be given by $P_n^{PM} = \sum_m T_{m,n} P_n^{e\dot{q}}(\lambda_i)$, which is not an equilibrium state, instead of the thermal population P_n^h . This change will affect the heat exchange and the work done during the Otto cycle. The origin of this difference lies on the measurement process, which has more free parameters than the two baths protocol, while the thermal fluctuations are responsible for the work and heat exchanged in the latter one.

For simplicity purposes, we will restrict the measurement process to a projective measurement. A possible set of projective measurement operators for a three-level system is given by:

$$M_1 = |\psi_1\rangle\langle\psi_1|, M_2 = |\psi_2\rangle\langle\psi_2|, M_3 = |\psi_3\rangle\langle\psi_3|, \quad (4.1.2.1)$$

where

$$|\psi_1\rangle = \cos\theta \sin\phi e^{i\chi} |0\rangle + \sin\theta \sin\phi e^{i\psi} |1\rangle + \cos\phi |2\rangle, \quad (4.1.2.2)$$

$$|\psi_2\rangle = \cos\theta \cos\phi e^{i\chi} |0\rangle + \sin\theta \cos\phi e^{i\psi} |1\rangle - \sin\phi |2\rangle, \quad (4.1.2.3)$$

$$|\psi_3\rangle = \sin\theta e^{i\chi} |0\rangle - \cos\theta e^{i\psi} |1\rangle, \quad (4.1.2.4)$$

with $\theta, \phi, \chi \in [-\pi, \pi]$ and $\psi \in [-\pi/2, \pi/2]$. This set of projectors belongs to the $SU(3)$ group and

can be used to make a generic projective measurement in any direction [153]. We can rewrite the projective operators in the matricial form using the computational basis as

$$M_1 = \begin{bmatrix} \cos^2(\theta) \sin^2(\phi) & e^{-i(\psi-\chi)} a(\theta, \phi) & e^{i\chi} b(\theta, \phi) \\ e^{i(\psi-\chi)} a(\theta, \phi) & \sin^2(\theta) \sin^2(\phi) & e^{i\psi} c(\theta, \phi) \\ e^{-i\chi} b(\theta, \phi) & e^{-i\psi} c(\theta, \phi) & \cos^2(\phi) \end{bmatrix}, \quad (4.1.2.5)$$

$$M_2 = \begin{bmatrix} \cos^2(\theta) \sin^2(\phi) & e^{-i(\psi-\chi)} d(\theta, \phi) & -e^{i\chi} b(\theta, \phi) \\ e^{i(\psi-\chi)} d(\theta, \phi) & \sin^2(\theta) \sin^2(\phi) & -e^{i\psi} c(\theta, \phi) \\ -e^{-i\chi} b(\theta, \phi) & -e^{-i\psi} c(\theta, \phi) & \sin^2(\phi) \end{bmatrix}, \quad (4.1.2.6)$$

$$M_3 = \begin{bmatrix} \sin^2(\theta) & -\frac{1}{2} e^{-i(\psi-\chi)} \sin(2\theta) & 0 \\ -\frac{1}{2} e^{i(\psi-\chi)} \sin(2\theta) & \cos^2(\theta) & 0 \\ 0 & 0 & 0 \end{bmatrix}, \quad (4.1.2.7)$$

where

$$a(\theta, \phi) = \frac{1}{2} \sin(2\theta) \sin^2(\phi), \quad (4.1.2.8)$$

$$b(\theta, \phi) = \frac{1}{2} \cos(\theta) \sin(2\phi), \quad (4.1.2.9)$$

$$c(\theta, \phi) = \frac{1}{2} \sin(\theta) \sin(2\phi), \quad (4.1.2.10)$$

$$d(\theta, \phi) = \frac{1}{2} \sin(2\theta) \cos^2(\phi). \quad (4.1.2.11)$$

Unlike the two-baths case, where we have two temperatures as free parameters, in this case we must deal with only one temperature given by $\beta_c = 1/k_B T_c$. However, we gain four new free parameters from the measurement process instead: θ, ϕ, χ and ψ . The general expressions for the heat, work and efficiency become very cumbersome, so we will present just the general efficiency equation. For some chosen angles we can simplify the efficiency as follows:

$$\eta = \frac{(\alpha - \gamma e^{2B_i} + \delta e^{B_i+J})(B_f - B_i) + \sigma J}{(\alpha - \gamma e^{2B_i} + \delta e^{B_i+J})B_f + (\omega + \lambda e^{2B_i} - \zeta e^{B_i+J})J}, \quad (4.1.2.12)$$

where $\alpha, \gamma, \delta, \lambda, \omega, \zeta, \sigma$ are all functions of the measurement angles. Unfortunately these functions are too complicated and do not bring any physical insight about the measurement process. The only way to simplify them is to set values to the angles in order to obtain numerical results of the efficiency in terms of $B_{i(f)}, \beta$ and J . For example, if we set the parameters as $\theta = \phi = 0.7\pi$, $\psi = \chi = 0.5\pi$ and $\beta = 1$, we obtain:

$$\eta_1 = \frac{(0.19 - 1.17e^{2B_i} + 0.97e^{J+B_i})(B_f - B_i) + 9.1 \times 10^{-16} e^{J+B_i} J}{(0.19 - 1.17e^{2B_i} + 0.97e^{J+B_i})B_f + (0.025 + e^{2B_i} - 1.02e^{J+B_i})J}. \quad (4.1.2.13)$$

As expected, we recover the qubit efficiency η_0 for $J = 0$. Also, we can get an efficiency greater or less than the two-baths efficiency (η_T) for $J \neq 0$, depending on the angles we choose for our measurement. In fig. 4.4 we show the efficiency for the qubit case (dotted red line), the qutrit in the two-baths model (dotted black line) and for three different measures settings (solids lines).

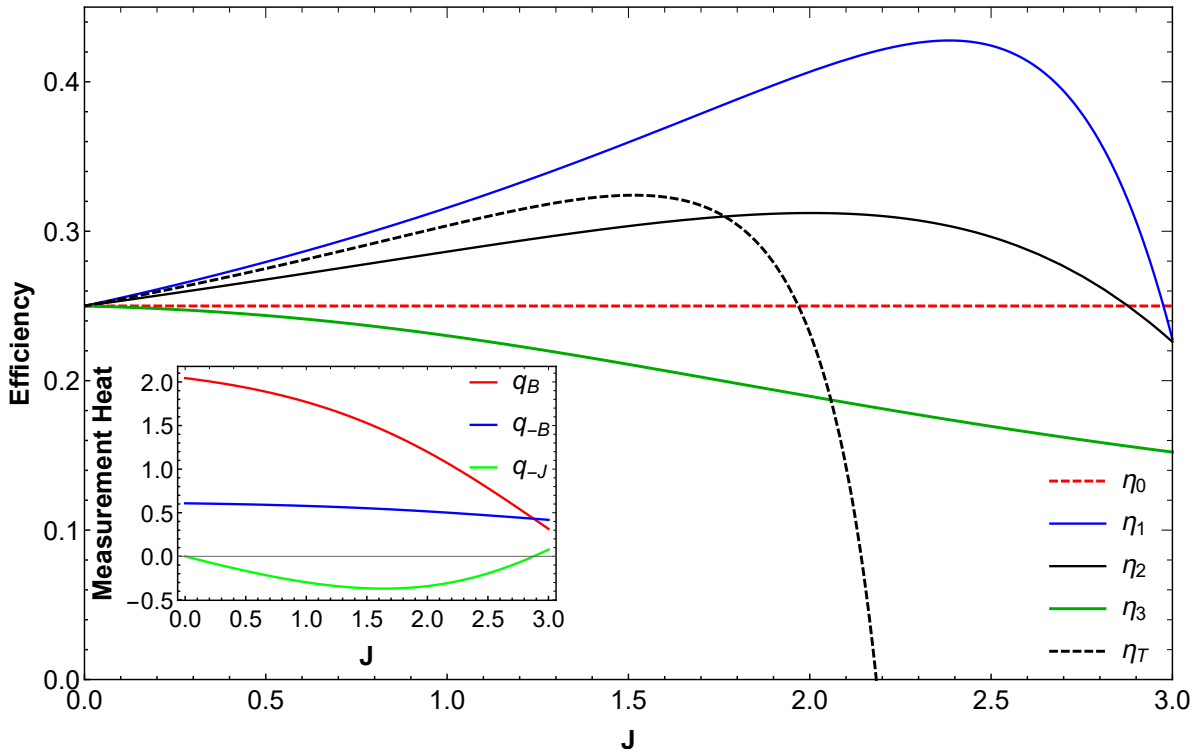


Figure 4.4: Efficiency of measurement-based quantum heat engine for a qutrit. Here we have: (Blue) η_1 with $\theta = \phi = 0.7\pi$ and $\psi = \chi = 0.5\pi$, (Solid black) η_2 with $\theta = \phi = \chi = 0.7\pi$ and $\psi = 0.5\pi$; (Green) η_3 with $\theta = \phi = \chi = \psi = 0.3\pi$; (Dashed black) Two-baths quantum Otto engine efficiency. (Inset) Energy flowing through each energy level for the case η_2 .

It is clear from the fig.(4.4) that there are all possible outcomes for the efficiency. It can be greater than the two-baths model efficiency, e.g., η_1 which is measured in the directions $\theta = \phi = 0.7\pi$ and $\psi = \chi = 0.5\pi$. It also can be lower than η_T but greater than η_0 , e.g., η_2 with the angles given by $\theta = \phi = \chi = 0.7\pi$ and $\psi = 0.5\pi$. It is possible to have an outcome where the efficiency is even lower than the qubit limit, e.g., η_3 measured for the angles $\theta = \phi = \chi = \psi = 0.3\pi$.

The inset figure shows the flowing energy for the efficiency η_2 with its respective measurement angles. We can see, once again, that in the region where the q_{-J} is negative, the efficiency becomes greater than the qubit efficiency limit. The same is valid for all the three measurement curves showed in this figure and any other possible choice of measurement. The opposite is also true. In the η_3 case, for example, the heat flow through the $-J$ level is in the same direction as the overflow, and the efficiency is lower than η_0 . In addition, one important result to notice here is the fact that we can achieve an efficiency greater than the two-baths at least for one good choice of angles.

Unfortunately, the increase in efficiency is not accompanied by an increase of the work extraction. As one can see in fig.(4.5) the most efficient among the five ones presented, η_1 , does not give us the greater work extraction, even though it has an efficiency greater than the efficiency η_2 , which extract more work.

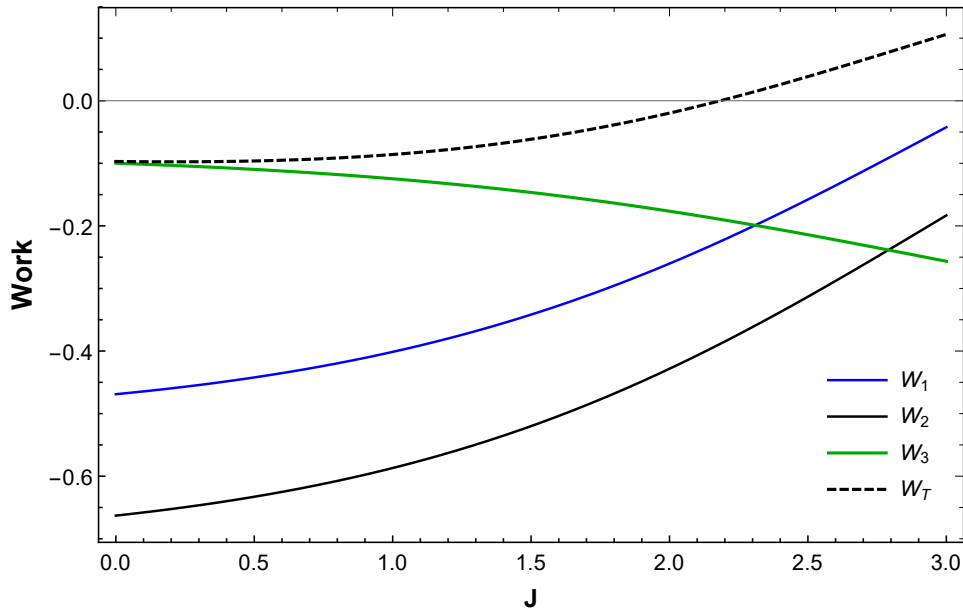


Figure 4.5: Work of measurement-based quantum heat engine for a qutrit. Here we have the work done for each one of the efficiencies presented in fig.(4.4).

Another interesting result is that, from all angles that we have looked at, the range of values of J where the system works as an engine and where the efficiency increases is wider than in the two-baths model. For instance, in the measurement-based model, the efficiency can increase for positive and negative values of J , while in the two-baths model the efficiency does not increase over the qubit limit for values of $J < 0$.

In fig.(4.6) we made a contour plot of the efficiency as a function of the angle parameters and the energy level J . In fig.(4.6-a) we set the efficiency as a function of the angles such as $\theta = \phi = \chi \in [0, \pi]$ and J for a fixed value of $\psi = \pi/2$ at the inverse temperature $\beta_c = 1$, whereas fig.(4.6-b,c,d) shows the efficiency for the same angles and J at different inverse temperatures: $\beta_c = 1$, $\beta_c = 0.25$ and $\beta_c = 4$, respectively. The result is that the efficiency, for this set of parameters values, becomes robust against temperature changing.

In order to maximize the efficiency, we note that if one sets the angles ψ and $\chi \in [0, \pi]$, such that $\psi = \chi = \pi/2$, due to the symmetry of these parameters in the measurement process, the efficiency can be increased until 1. Even though the qutrit efficiency can achieve the unit efficiency, it does not violate the second law of thermodynamics, since this engine does not work between two thermal baths. This measurement-based engine only requires one thermal bath and one measurement process, which can be seen as a non-thermal bath, while the second law requires, at least, two thermal baths. In this sense, the second law is not define for this case. Some work has been done to find bound to engines working with non-thermal baths [154], but it is not clear how it is applied to this case. Even though the second law is not applied here, we still observe that the energy Q_M is not all converted in work during the cycle. Some energy Q_c is released in the cold reservoir (see fig. 4.7).

In fig.(4.8) we can analyse the system's energy and population for these specific parameters that achieves $\eta = 1$. Note that, before the measurement process, the system is effectively in a two state configuration, since the population of the $+B$ energy level is almost zero. The population of the $-B$ and $-J$ energy levels becomes closer while J increases. After the measurement process, these populations remain the same for all values of J . So the system starts to behave as if it were in contact with an infinite temperature bath, with both the two states with the same population. In

the limit where the $-B$ and $-J$ levels became almost degenerated, the measurement won't affect the state. Without affecting the system, there won't be any work done $W = 0$.

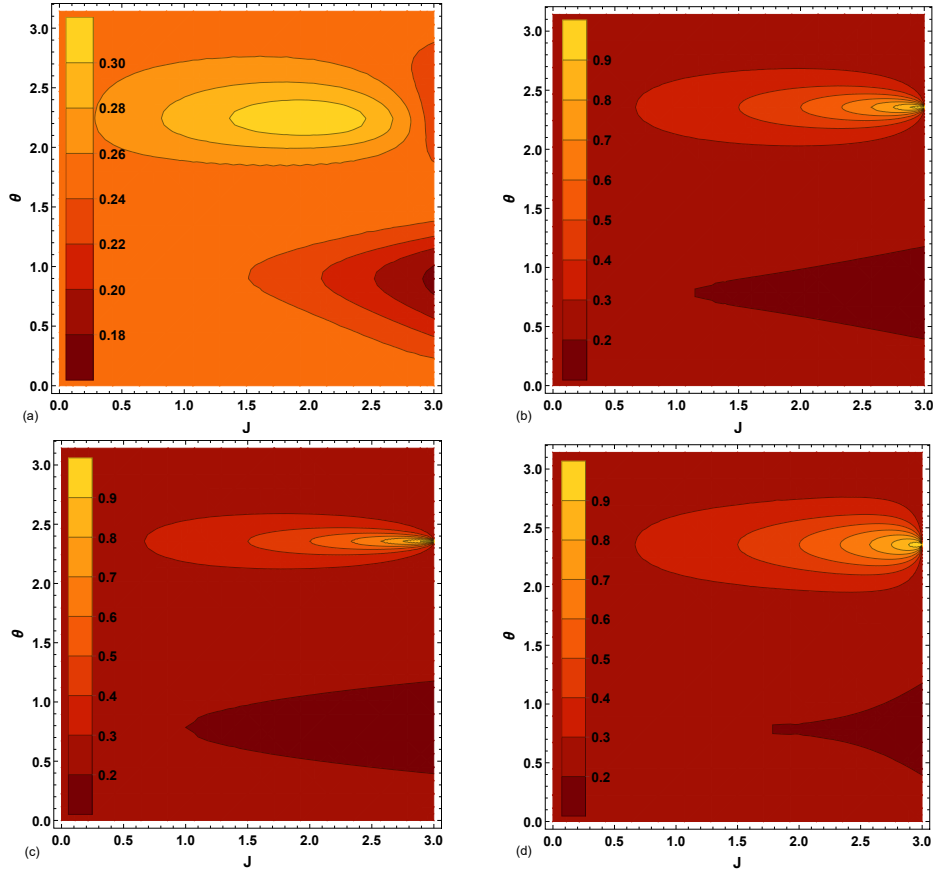


Figure 4.6: Contour plot of the qutrit efficiency in a measurement-based heat engine. (a) $\theta = \phi = \chi \in [0, \pi]$, J for a fixed angle $\psi = \pi/2$ and $\beta = 1$. (b),(c) and (d) $\theta = \phi \in [0, \pi]$ and J for fixed angles $\psi = \chi = \pi/2$ and $\beta = 1$, $\beta = 0.25$, $\beta = 4$, respectively.

The measurement-based protocol presents some advantages over the conventional two-baths model. It not only benefits from the efficiency boost for larger values of J , but also it can surpass the two-baths efficiency for a measurement apparatus which can be precisely controlled by the experimenter. If this precise control is possible, one can maximize the efficiency by maximizing the population difference ΔP_n of the energy level that does not contribute to the work, $-J$ level in our case, in order to maximize the value of q_n . Even though the measurement process is still random process, since there is no feedback control, it is less random than the heat exchange between both heat baths at different temperatures, which cannot be controlled in any way.

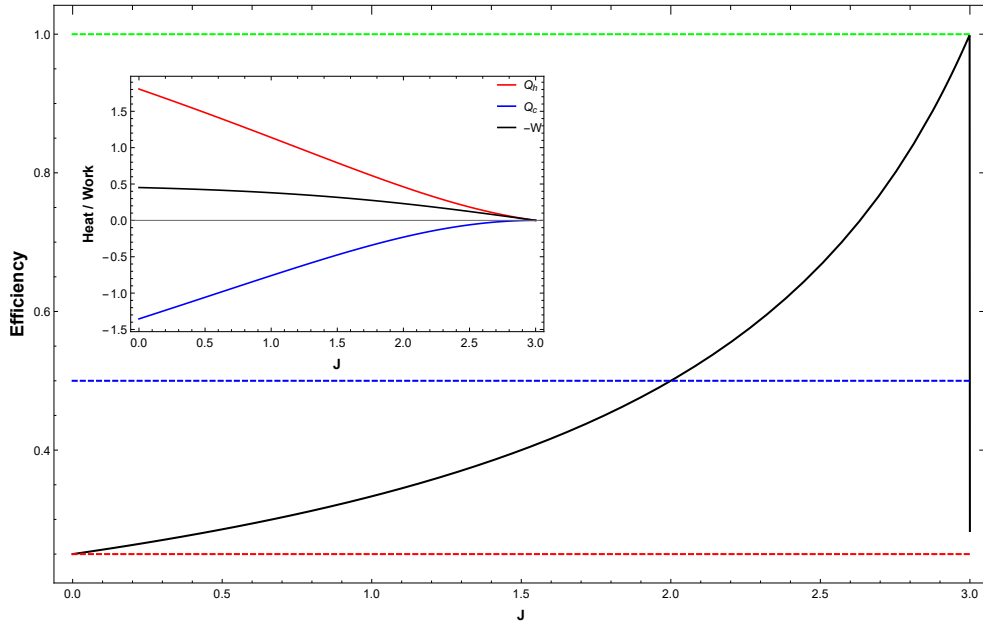


Figure 4.7: Efficiency of a qutrit system for the measurement angles given by $\psi = \chi = 0.5\pi$ and $\theta = \phi = 0.75005\pi$ (Black), Carnot efficiency for $T_h = 2$ and $T_c = 1$ (Blue) and unit efficiency limit (Green). (Inset) Work (Black) and heat exchanged (Red and Blue) during the cycle for this set of parameters.

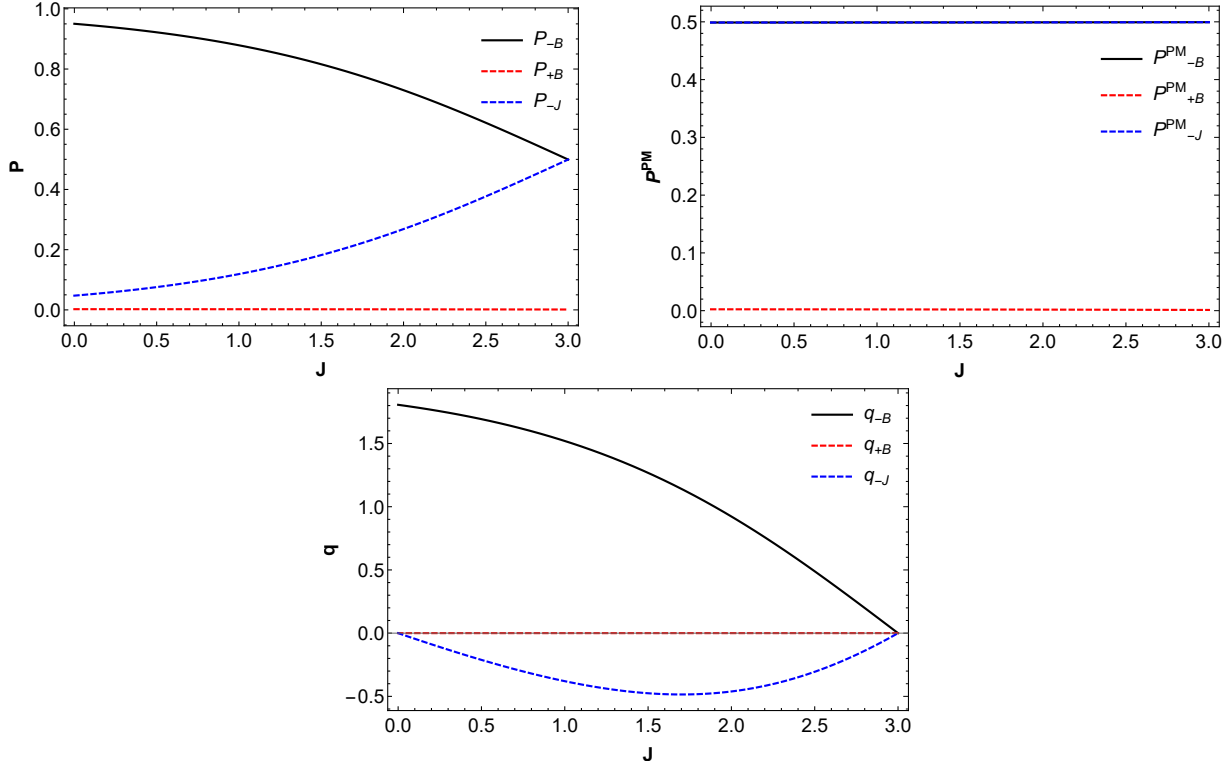


Figure 4.8: Energy and population structure for the qutrit system: Initial (cold) thermal population for $\beta = 1$ (upper left). Population after the measurement process, third stroke of the cycle (upper right). Energy flowing through each energy level during the third stroke (bottom). All these functions are given for the same parameters of fig.(4.7).

4.2 Revisiting the Heisenberg model as QHE

The Heisenberg model with two qubits system as a quantum heat engine has already been studied in the literature [117, 152]. In the first one, the energy exchanged in each energy level, here defined as q_n , was interpreted as a local heat flowing into each one of the two qubits. In the second paper the mechanism behind the efficiency boost was not clear. In this section we will show the condition to observe an efficiency boost for the Heisenberg model in terms of the energy exchanged in each energy level, as we did in the qutrit case.

Let's consider the anisotropic Heisenberg model for two qubits system ruled by the Hamiltonian:

$$\mathcal{H}_{Hei} = J_{xy}(\sigma_x^1 \sigma_x^2 + \sigma_y^1 \sigma_y^2) + J_z \sigma_z^1 \sigma_z^2 + B(\sigma_z^1 + \sigma_z^2), \quad (4.2.0.1)$$

where J_{xy} is the interaction of the spins in the xy -plane, J_z is the interaction in the z -direction and B is the external magnetic field and $\sigma_i^{1(2)}$ are the Pauli matrices associated with the particle 1(2). The eigenvalues and eigenvectors are given in the table 4.2

Eigenvalues	Eigenstates
$2B$	$ 00\rangle$
$2(J_{xy} - J_z)$	$(01\rangle + 10\rangle)/\sqrt{2}$
$-2(J_{xy} + J_z)$	$-(01\rangle - 10\rangle)/\sqrt{2}$
$-2B$	$ 11\rangle$

Table 4.2: The three eigenvalues of the Hamiltonian \mathcal{H}_{Hei} with their associated eigenvectors.

Unlike the qutrit case, there are two energy levels which do not contribute to the total work. In this sense, eq.(4.1.0.10) can be rewritten as

$$\frac{\eta}{\eta_0} = 1 - \frac{q_1 + q_2}{Q_{h(M)}}, \quad (4.2.0.2)$$

where q_1 and q_2 are the energy exchanged in the energy level associated with the eigenvalue $2(J_{xy} - J_z)$ and $-2(J_{xy} + J_z)$, respectively. When $q_1 + q_2 < 0$, there will be an efficiency boost. This means that, at least, one of these energy levels will have the energy exchanged in the opposite direction ($q_{1(2)} < 0$).

If $J_{xy} = J_z$, there will be basically three energy levels. Then, we recover eq.(4.1.0.10) for energies given by: $2B, 0, -4J, -2B$. This leads to $\eta/\eta_0 = 1 - q_2/Q_{h(M)}$. We shall see next the evaluation of the efficiency of quantum Otto cycle for both two-baths and measurement-based protocols.

4.2.1 Two-bath model with Heisenberg interaction

For a QHE working between two thermal baths at temperatures T_h and T_c , we can calculate the efficiency as

$$\eta_T = \frac{(B_f - B_i)}{2\mathcal{X}} e^{-2J_{xy}} [2e^{2J_{xy}} (e^{2B_f} - e^{-4B_i}) - e^{B_f + J_{xy} + J_z} (e^{4J_{xy}} - 1) (1 + (e^{2J_{xy}} + e^{2(B_i + J_z)} (e^{2J_z} - 1) (1 + e^{4J_{xy}}))), \quad (4.2.1.1)$$

where

$$\begin{aligned} \mathcal{Z} = & B_f(e^{2B_f} - e^{4B_i}) + e^{2B_f+J_z}(1 + e^{4B_i})(J_z \cosh(J_{xy}) + J_{xy} \sinh(J_{xy})) - 2e^{B_f+2B_i+J_z}(B_f \cosh(J_{xy}) \sinh(2B_i) \\ & + e^{2J_z} J_{xy} \sinh(J_{xy}) + e^{J_z}(\cosh(2J_{xy})(J_z \cosh(B_f) - B_f \sinh B_f) + J_{xy} \cosh B_f \sinh 2J_{xy})). \end{aligned} \quad (4.2.1.2)$$

This equation becomes the same as the one analysed in reference [117] when $J_{xy} = J_z$. Let's analyse eq.(4.2.0.2) for the two possible cases: $J_{xy} = J_z$ and $J_{xy} \neq J_z^3$.

In the first case, $J_{xy} = J_z = J$, this system can be interpreted as a quantum Otto cycle working with a three-level system. The only negative term of Q_h will be given by the energy level $-4J$. To illustrate the effect of having a three-level system with one energy level that does not depend on the magnetic field, we plot the efficiency and the energy exchanged in this level in fig.4.9. One can see that the energy exchanged in the $-4J$ energy level is negative, while the efficiency is greater than η_0 . This is in complete agreement with eq.(4.2.0.2), where, $q_1 = 0$. This shows that the eq.(4.2.0.2) is in total agreement with eq.(4.1.0.10).

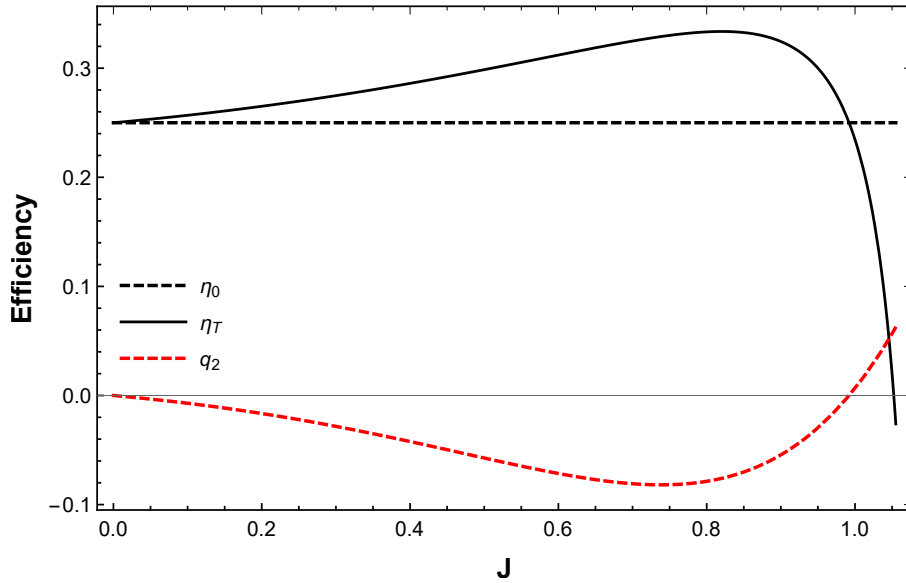


Figure 4.9: Efficiency of two qubits system for a QHE working between two thermal reservoirs (Black). Single qubit efficiency (Dashed black line). Energy exchanged from the system to the bath in the $-4J$ energy level (Red).

For the case $J_{xy} \neq J_z$, we can choose any values of J_{xy} and J_z since it does not cross any energy levels. For simplicity purposes, we show the cases where $J_z = 0$ and then $J_{xy} = 0$. In fig.4.10 we can see how the total energy exchanged in each energy level that is dependent on J_{xy} and J_z is negative while the efficiency is greater than η_0 . This shows that the mechanisms behind the efficiency boost are due to the energy exchanged in the opposite direction in at least one of the energy levels.

³Recall that energy crossing can not happen.

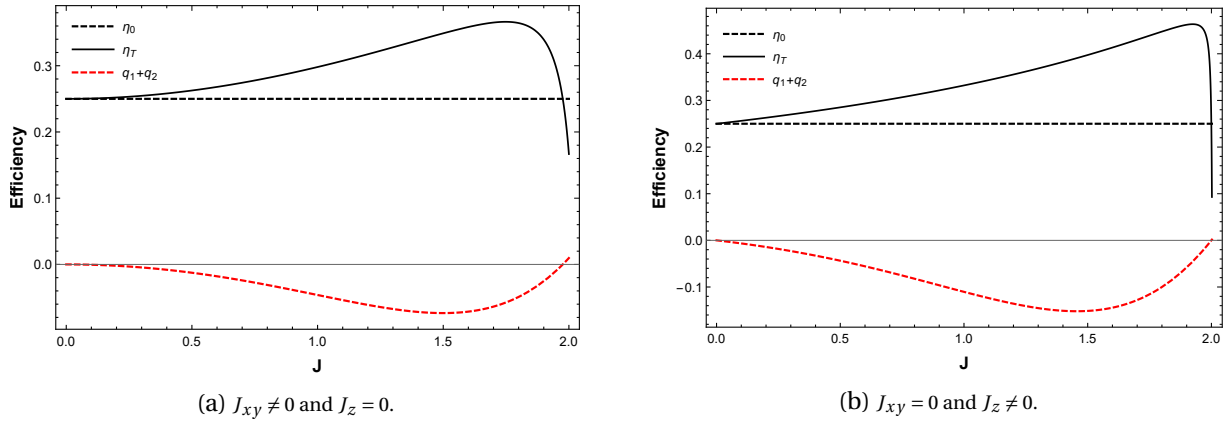


Figure 4.10: Heisenberg QHE efficiency (Black). The red line is the sum of the two energy flux in the energy levels that are dependent on J . Dashed line is the single qubit efficiency.

4.2.2 Measurement-based with Heisenberg model

In this section we will analyse the same process that we did in the qutrit quantum heat engine based on a measurement process. For a two qubit system, we chose the projective measurement on the spin direction of each qubit of the system. For this case, the projectors are given by

$$\begin{aligned}
 M_1 &= |+\rangle\langle +| \otimes |+\rangle\langle +|, \\
 M_2 &= |+\rangle\langle +| \otimes |-\rangle\langle -|, \\
 M_3 &= |-\rangle\langle -| \otimes |+\rangle\langle +|, \\
 M_4 &= |-\rangle\langle -| \otimes |-\rangle\langle -|,
 \end{aligned} \tag{4.2.2.1}$$

where $| \pm^n \rangle \langle \pm^n |$ are the projectors for the observable $\vec{\sigma} \cdot \hat{n}$ for one spin and $| \pm^m \rangle \langle \pm^m |$ are the projectors for the observable $\vec{\sigma} \cdot \hat{m}$ for the other one. From these operators, we can measure each qubit in any direction.

In reference [152], they studied this same system with this projective measurement for the case $J_{xy} = J_z$ without explaining the mechanism behind the efficiency boost. We are now able to show that their result obeys the eq.(4.2.0.2).

As an example, in fig.(4.11) we show the three same efficiencies studied in the reference [152] for $J_{xy} = J_z = J$. The inset figure shows the energy exchanged in each measurement direction. As expected, the eq.(4.2.0.2) is still valid for the measurement-based heat engine. One can see that for the xy and xx-direction, the efficiency becomes smaller than the qubit efficiency at the same point. It leads to the same value of J where $q_{xy} + q_{xx}$ becomes positive, according to eq.(4.2.0.2).

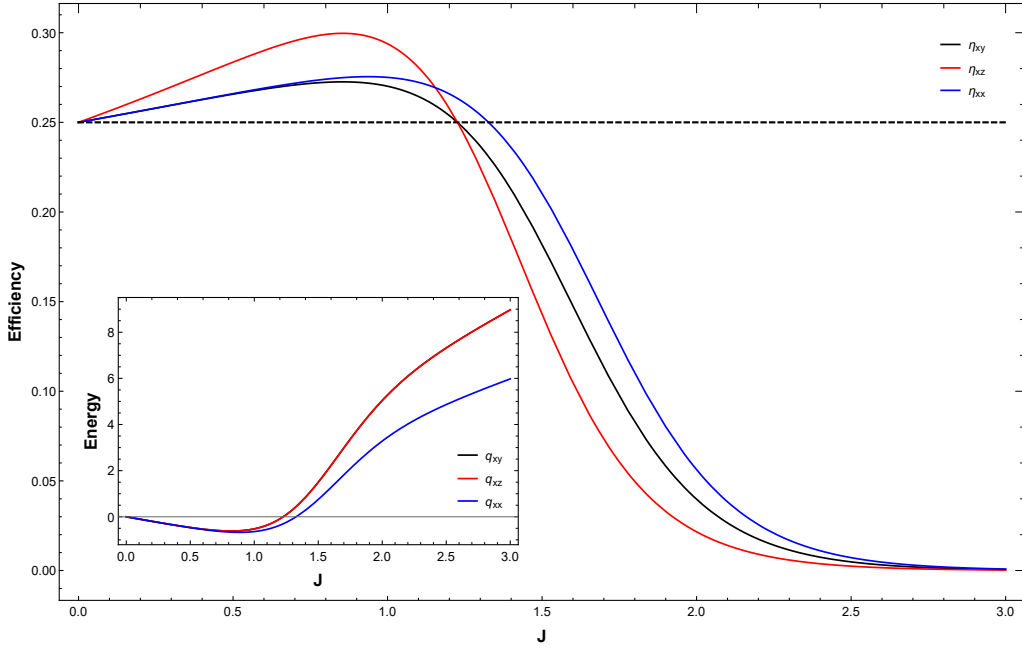


Figure 4.11: Efficiency of two qubits system for a single-bath engine. (Black) η_{xy} is the efficiency in the x-direction measurement of one spin and in the y-direction for the other one. The same for the efficiency η_{xz} (Red) and η_{xx} (Blue). The dashed line is the single qubit efficiency. (Inset) Energy flowing in the energy levels of $-4J$ in each direction.

As we did before, we can analyse the same system for different strengths of the interaction. Just like before, let's consider two cases: $J_{xy} \neq 0, J_z = 0$ and $J_{xy} = 0, J_z \neq 0$.

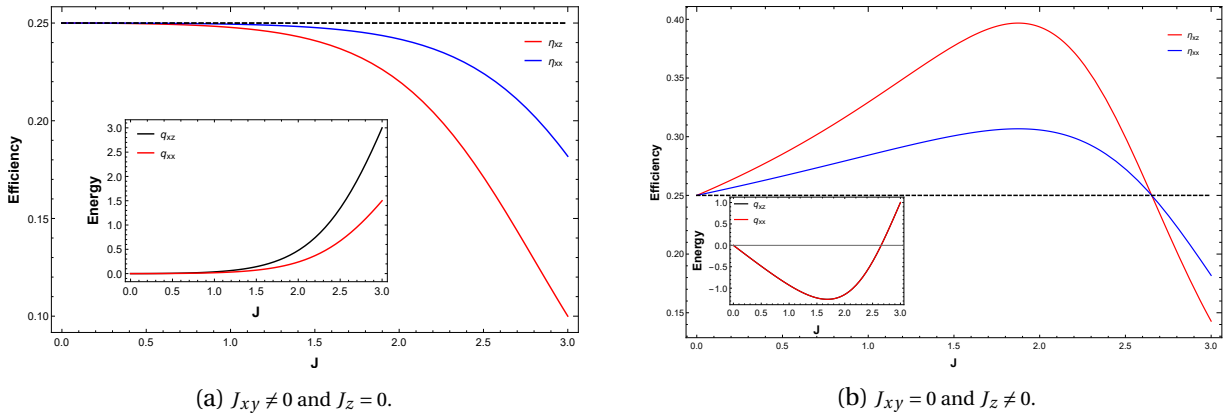


Figure 4.12: Heisenberg measurement QHE efficiency. The efficiencies are given in two directions η_{xz} (Red) and η_{xx} (Blue). The inset figure shows the energy exchanged in each energy level that is dependent of J_{xy} or J_z

As one can see clearly from the fig.4.12(a), the case where $J_z = 0$ does not show any boost on the efficiency. Thus, the total energy exchanged in the two energy levels that are dependent on J_{xy} and J_z is positive, $q_1 + q_2 > 0$. However, when $J_{xy} = 0$, $q_1 + q_2 < 0$. Then, there is a boost in the efficiency in a small region of J_z .

As we wished to show, the validity of eq.(4.1.0.10) can be extended to more than three energy level system, given by eq.(4.2.0.2). This equation is more general because it can be reduced to a three-level case when we rescale the energy of the system, e.g., isotropic Heisenberg Hamiltonian for two spins. But even in the case where no three-level rescale can be done, it is still valid while the condition $q_1 + q_2 < 0$ holds. In addition, no arguments based on quantum properties, as entanglement and quantum coherence, was necessary to explain the efficiency boost.

Conclusion

In the present work we studied basic processes of thermodynamics in the quantum regime. We first reviewed the extension of fundamental concepts, properties and laws of classical thermodynamics, accepted in the literature so far, to the quantum theory realm. As an important application of such fundamental properties, we introduced a brief review of one of the most important branches of quantum thermodynamics, the study of thermal heat engines. We also reviewed the quantum Carnot cycle which, just like its classical counterpart, has the same efficiency when it is working between two thermal heat baths at different temperatures. It is also still the upper bound to the efficiency of other quantum cycles [35]. Next we showed the quantum Otto heat cycle, which is extensively studied in quantum thermodynamics [34, 117, 118, 119, 120, 121]. We also gave a detailed description of a new proposal presented by Talkner et. al in 2017 [55], where the measurement process without feedback control replaces the hot heat bath.

Our goal in this work was to study the efficiency of the quantum Otto cycle in two different models, from the traditional two-baths setup and the new measurement-based protocol. The idea behind this study is to understand the mechanism responsible for the boost or reduction of the efficiency during a cycle. Since entanglement and other quantum features are usually used to explain this mechanism in certain situations, we first studied a simple three-level quantum system which is free of any entanglement or any other quantum correlation that could be used to justify the increase in the efficiency. In doing so, we proposed an interpretation for this mechanism that deals with the energy exchanged in each one of the energy levels of the system. We showed that in our model, only the heat exchanged through the energy levels $\pm B$, that depend on the external parameter of the Hamiltonian, will contribute to the work. On the other hand, the energy exchanged in the energy level $-J$, which does not contribute to the work, is responsible for the efficiency boost. This enhancement will be observed whenever the energy exchanged through the J -energy level flows in the opposite direction, i.e., from the cold to the hot bath. We believe that this phenomenon can be justified due to the fact that the system is not in an equilibrium state after the adiabatic process, and is driven away even more after the measurement. This mechanism is valid for both two-baths and measurement-based quantum Otto engines. In addition, this interpretation does not require any quantum correlations to be valid, since it just depends on the energy level structure of the system under consideration. It also must presents one energy level with some fixed parameter that does not change during the adiabatic process, while the other energy levels change without this fixed parameter dependence. Finally, we showed that this same mechanism can explain the efficiency boost in a system of two coupled qubits. In this case, the opposite energy flux must happen in, at least, one of the energy levels that does not contribute to the total work. Therefore, no quantum correlation is necessary to explain the higher efficiency in

this case.

In future projects, we intend to study more carefully the origin of this mechanism for general systems. We also intend to study more complex systems and try to understand if any quantum correlations can be useful in this case. Also, we intend to study more realistic systems, with the master equation approach to include any imperfection and perturbations of the environment, using this approach to revisit the work done here and analyse from a way more realistic perspective.

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