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**Autonomous quantum Maxwell's demon
using superconducting devices**

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**Autonomous quantum Maxwell's demon
using superconducting devices**

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Physics at the Instituto de Física de São Carlos, Uni-
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To all the demons that haunt, not only the castle of physics, but also our extraordinary and delicate human minds.

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“Thoroughly conscious ignorance is the prelude to every real advance in science.”

James Clerk Maxwell

ABSTRACT

MARTINS, G. F. **Autonomous quantum Maxwell's demon using superconducting devices.** 2019. 90p. Dissertation (Master in Science) - Instituto de Física de São Carlos, Universidade de São Paulo, São Carlos, 2019.

During the last years, with the evolution of technology enabling the control of nano-mesoscopic systems, the possibility of experimentally implementing a Maxwell's demon has aroused much interest. Its classical version has already been implemented, in photonic and electronic systems, and currently its quantum version is being broadly studied. In this context, the purpose of this work is the development of a protocol for the implementation of the quantum version of an autonomous Maxwell's demon in a system of superconducting qubits. The system is composed of an Asymmetrical Single-Cooper-Pair Transistor, ASCPT, which has its extremities in contact with heat baths, such that the left one has a lower temperature than the right one. And of a device of two interacting Cooper-Pair Boxes, CPB's, named as an ECPB, for Extended Cooper-Pair Box. The ECPB is also in contact with a heat bath and possess a genuine quantum feature, entanglement, being described by its antisymmetric and symmetric states, that couple capacitively to the ASCPT with different strengths. A specific operating regime was found where the spontaneous dynamics of the tunneling of Cooper pairs through the ASCPT, will led to a heat transport from the bath in contact with the left extremity of the ASCPT to the bath at the right. And so, as in Maxwell's original thought experiment, the demon, which is composed by the ECPB and the island of the ASCPT, mediates a heat flux from a cold to a hot bath, without the expense of work. However as expected, the violation of the 2nd law of thermodynamics does not occur, as during the dynamics heat is also released to the bath in contact with the ECPB, compensating the decrease of entropy that occurs in the baths in contact with the ASCPT.

Keywords: Maxwell's demon. Superconducting devices. Open quantum systems.

RESUMO

MARTINS, G. F. **Demônio de Maxwell quântico em um sistema de dispositivos supercondutores**. 2019. 90p. Dissertação (Mestrado em Ciências) - Instituto de Física de São Carlos, Universidade de São Paulo, São Carlos, 2019.

Nos últimos anos, com a evolução da tecnologia que permite o controle de sistemas nano-mesoscópicos, a possibilidade de se implementar um demônio de Maxwell despertou muito interesse. A sua versão clássica já foi realizada experimentalmente com sucesso em sistemas fotônicos e eletrônicos e atualmente a versão quântica tem sido amplamente estudada. Neste contexto, o objetivo deste trabalho é desenvolver um protocolo para a implementação de uma versão quântica de um demônio de Maxwell autônomo utilizando dispositivos supercondutores. O sistema é composto por um Asymmetrical Single-Cooper-Pair Transistor, ASCPT, que possui as suas extremidades em contato com banhos térmicos, sendo que o banho à esquerda possui uma temperatura inferior ao da direita. E por um dispositivo composto por dois Cooper-Pair Boxes, CPB's, interagentes, denominado ECPB, sigla para Extended Cooper-Pair Box. O ECPB também se encontra em contato com um banho e possui uma característica genuinamente quântica, emaranhamento, sendo descrito por seus estados antissimétrico e simétrico, que se acoplam capacitivamente ao ASCPT com intensidades distintas. Encontrou-se que em um regime de operação específico a dinâmica espontânea de tunelamento de pares de Cooper ao longo do ASCPT origina o transporte de calor do banho à esquerda do ASCPT, ao banho à direita. Desta forma, assim como proposto originalmente por Maxwell, o demônio, composto pelo ECPB e pela ilha do ASCPT, media um fluxo de calor de um banho frio para um banho quente, sem a realização alguma de trabalho. Contudo como esperado, a violação da 2ª lei da termodinâmica não ocorre, já que durante a dinâmica calor é liberado ao banho em contato com o dispositivo de CPB's, compensando a diminuição de entropia que ocorre nos banhos em contato com o ASCPT.

Palavras-chave: Demônio de Maxwell. Dispositivos supercondutores. Sistemas quânticos abertos.

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Chapter 1

Introduction

Physics aims to understand, describe and predict all the different and intriguing phenomena that occur in our universe. From mechanics, to electromagnetism and thermodynamics, all physical theories possess their unique set of laws, which may be accurate only in a given regime of validity, but nonetheless explain the events observed in nature which are restricted to occur in such regime. So, it is not surprising that if a situation is conceived in which one of those laws is apparently violated, the attention of the scientific community is dragged into trying to solve the paradox created. That theory on specific may not yet have been correctly formulated, and there is space to the development of new laws and even new theories. Or there is some subtlety in the analysis of the situation itself, and the law actually is not violated.

One of the most striking examples of such “violation” in natural laws is the Maxwell’s demon. The thought experiment imagined by Maxwell entails in breaking the 2nd law of thermodynamics, a theory that has undergone extensive experimental tests, always reassuring its validity. If such demon was real, a perpetual motion machine of the second type could be created and a process that has as sole effect to convert heat totally into work would be established. That is, the demon would be able to decrease the entropy of a system without the realization of work on it. Unfortunately, the construction of macroscopic heat engines with no upper limit for their efficiency is not possible, as it was shown that the demon does not actually violate the 2nd law. That is, there is a subtlety: to be able to act in the described way, the demon will also undergo an increase in its entropy, compensating the decrease of entropy it caused in the system in which it was acting.

However, Maxwell’s demon continues to intrigue and challenge scientists during more than 150 years from its original conception. It may not consist in a real threat to the 2nd law, but it has helped to shed light upon very important physical concepts, being one of them the link between information and thermodynamics. So, given its relevance and the evolution of technology, it was expected that the possibility of experimentally implementing a Maxwell’s demon would spark the interest of at least part of the scientific community. And so, in the last years, classical demons have

been successfully implemented in photonic and electronic devices, while its quantum experimental version has also been widely investigated.

The work here developed fits perfectly in the current scientific context, as it presents an implementation of an autonomous quantum Maxwell's demon using superconducting devices. And so, this dissertation is structured as follows: in Chapter 2 a short introduction on the history of Maxwell's demon is addressed. The original thought experiment conceived by Maxwell is described and all its numerous different versions that have appeared during the years are also presented. Special attention is given to Szilard's engine, which enabled the introduction of a more simplified analysis for the working of the demon. Also, the solution to the apparent paradox created by the demon is discussed. This solution is due to Bennett, who applied Landauer's principle to the specific case of the demon's problem. The proofs of Landauer's principle, for the classical and quantum cases, are addressed. For last, the theoretical work developed on the quantum version of the demon is explained. In Chapter 3 the focus is given to experimental implementations of Maxwell's demon that have been accomplished during the last years. The research developed by Pekola's group, *On-chip Maxwell's demon as an information-powered refrigerator* (1), that served as an inspiration for this work, is analyzed. Then, in Chapter 4, we present the result of this work, our autonomous quantum Maxwell's demon implemented using superconducting devices. The constituents of the device are discussed, and the dynamics and working of this demon are explained in large detail. It is worth mentioning in advance that the demon developed in this work is responsible for creating a heat flux from a cold to a hot bath, and that it presents a genuinely quantum characteristic, entanglement.

Chapter 2

A short history of Maxwell's demon

The thought experiment that gave origin to the concept of Maxwell's demon, and all the subsequent developments made on this topic during more than 150 years of its existence, always sparked the interest of the scientific community. In this Chapter, the story behind the demon, from its “birth” to its “exorcism,” and the fundamental concepts underlying its mechanism, are addressed and discussed.

2.1 The 2nd law of thermodynamics

Thermodynamics underwent great development during the 19th century, while steam engines started to be widely used. The Watt steam engine, invented at the end of the 18th century, was one of the driving forces of the industrial revolution, a practical demonstration that heat leads to the ability to produce work. However, the connection between heat and energy was not yet made clear, with different hypotheses trying to explain the nature of heat itself. One of them is the now obsolete caloric theory, which stated that heat was a fluid substance flowing from hotter to colder bodies. Such a view reigned for a long time, despite the endorsement of prestigious scientists as F. Bacon and R. Hooke to the mechanical theory, which advocates that heat is directly related to the vibration movement of the particles that compose physical objects. The investigations on this topic lasted for more than half of a century and entailed in the formulation of the 1st law of thermodynamics. (2)

Important contributions were made by a miscellaneous of scientists, as the physician J. von Mayer that, inspired by the observation of diverse natural phenomena, came to the conclusion that “*Motion is converted to heat.*” (3,4) He was the first to calculate theoretically the value for the mechanical equivalent of heat using the reasoning that in a process at constant pressure, the heat used to produce the expansion is interconverted in work ⁱ. (5) The brewer J. Joule, who performed

ⁱ Mayer took experimental values on the specific heat and concluded that the fall of a weight from 365 m corresponds to the heating of the same weight of water from 0° C to 1° C. (4)

experiments on the heating of wires by currents, on the increase of temperature of a fluid caused by friction, and determined with great precision the mechanical equivalent of heat. As in his own words *“The amount of heat which is capable of heating one pound of water by 1 degree on the Fahrenheit scale [...] may be converted into a mechanical force which can lift 838 pounds to a vertical height of 1 foot.”*ⁱⁱ (4) In addition, Helmholtz, who presented a general formulation for what we know now as the principle of conservation of energy, stating that *“the quantity of force which can be brought into action in the whole of Nature is unchangeable, and can neither be increased nor diminished.”* (6) And hence made clear that perpetual motion machines of the first type cannot exist, as *“be impossible - by any combination of natural forces - to create life force continually from nothing.”*ⁱⁱⁱ (4, 7)

Still, a more precise statement of the 1st law was lacking. In 1850, R. Clausius defined a state function, U , denominated as energy and now acknowledged as internal energy. He stated that the differential of U was related to the heat and the work exchanged by a body with its environment, while undergoing a given process. Thus the 1st law of thermodynamics finally ceased to take on a vague form and turned to be described by a mathematical expression, so in its modern appearance:

$$\Delta U = Q - W \quad (2.1.1)$$

that is, the change on the internal energy, ΔU of a system is equal to the difference between the heat adsorbed by the system, Q and the work done by the system on its surroundings, W .

However, it is remarkable to note that, in mid-1820's, when even the 1st law had not yet been enunciated, S. Carnot was already developing a principle that would have wide impact in the field of thermodynamics^{iv}. He was interested in how to improve thermal engines, which have achieved a growing impact on all sectors of economy. In his work he described an ideal heat engine, composed of a piston, a working substance, a hot bath, T_H and a cold bath, T_C undergoing an idealized cycle. In modern terminology the Carnot cycle consists first of an isothermal expansion, carried out at T_H , and then of an adiabatic expansion, in which heat is converted into work. Subsequently an isothermal compression is carried out at T_C , and for last an adiabatic compression returns the working substance to its same macroscopic initial state. So, using arguments of reversibility, Carnot proved that there is no heat engine, regardless of its working substance, operating at the same temperature difference, that could possible extract more motive power^v than the ideal reversible one described

ⁱⁱ Mayer's did not receive much scientific recognition for his work, and even a debate on who should be credited the priority on the definition of the mechanical equivalent of heat arose between him and Joule. (4)

ⁱⁱⁱ Note that at that time the word force was used instead of energy, and the term “life force” mentioned by Helmholtz refers to the kinetic energy

^{iv} The work done by Carnot was of crucial importance on the later definition of the state function U (internal energy) by Clausius, that was previously mentioned. (4)

^v Carnot uses the term motive power to describe the maximum “duty” of an engine: its useful output. And as a believer of the caloric theory, at that time he could have never defined the maximum efficiency of his ideal engine.

by him. If such an engine existed, then a perpetual motion machine could be assembled, which was already known at the time not to be allowed in nature. That is, there is a fundamental limit preventing heat engines from being indefinitely improved. (2, 8)

Back in the 1850's, Clausius and W. Thomson, Lord Kelvin, further developed Carnot's statements, which led to the formulation of the 2nd law of thermodynamics. Therefore, in 1852 Lord Kelvin developed in his work the given axiom, known as the Kelvin statement of the 2nd law:

"It is impossible by means of inanimate material agency to derive a mechanical effect from a portion of matter by cooling it below the temperature of the coldest surrounding bodies." (9, 10)

that is, it is not possible to realize a process in nature that has the sole effect of removing heat from a body and producing an equivalent amount of work, see Fig. 2.1.1a.

By using his axiomatic form of the 2nd law, "Heat cannot pass by itself from a colder to a warmer body," Clausius arrives at the same conclusions as obtained by Carnot. (4) Also, later in 1854, using the absolute temperature scale devised by Lord Kelvin and the 1st law, Clausius finally defined the value of the efficiency of a Carnot cycle of an ideal gas, e_C , as:

$$e_C = 1 - \frac{T_C}{T_H} \quad (2.1.2)$$

In the same year, he slightly reshaped his statement for the 2nd law of thermodynamics, which assumed its notorious form:

"Heat can never pass from a colder to a warmer body without some other change, connected therewith, occurring at the same time." (10, 11)

that is, it is not possible to realize a process in nature that has the sole effect of transferring heat from a cold body to a hot body, see Fig. 2.1.1b. Clausius was then responsible for further developing a mathematical form for the 2nd law, known as Clausius's theorem:

$$\oint \frac{\delta Q}{T} \leq 0 \quad (2.1.3)$$

establishing that in a cyclic process the sum of all infinitesimal heat exchanges between a system and its surroundings, divided by the temperature of the surroundings, must be smaller or equal to zero, and the equality holds only if the process is reversible. He then coined the quantity $\delta Q/T$ as the infinitesimal variation of a state function, dS , named entropy. By using Eq. 2.1.3, he stated the principle of increase of entropy:

$$\Delta S \geq 0 \quad (2.1.4)$$

Figure 2.1.1 – Representation of the processes in nature that are not possible to be realized, as stated by the 2nd law of thermodynamics. The bodies in red are hot and the ones in blue are cold. Q represents the heat exchanged between a generic system and its environment. W represents the work done by the system. The gray dotted square represents the process that the system is undergoing.

Source: By the author

given that, the variation of entropy of a closed system is always positive or equal to zero, being zero only if the system undergoes a reversible process. In his own words:

“The entropy of the universe tends to a maximum.” (12)

Consequently, the 2nd law of thermodynamics imposes a fundamental limit on the processes that occur spontaneously in nature. As an example, assume an ideal gas initially restricted by a piston to the left partition of a container and in contact with a thermal bath. The piston is released, in such a way that the gas undergoes an isothermal expansion. So the gas moves the piston, and heat is extracted from the bath and totally converted into work. It is expected that the gas will expand until it occupies the whole volume of the container. If it was physically possible to the gas to spontaneously return to occupy only the left side of the container, the piston could be reinserted to its initial position, without the expenditure of work, and could be again released such that work was once more extracted from the expansion of the gas. A perpetual motion machine of the second type would be created, and a process that has as sole effect the total conversion of heat into useful work would be continuously occurring, violating the 2nd law.

The core of Maxwell’s thought experiment is exactly the possibility of conceiving an “intelligent being,” the demon, that would be able to return the gas initially from the whole volume to its initial left partition without the expenditure of any work. For this to be possible, the demon would collect information on the position and velocities of the particles of the gas and continuously trap them to the left side, until all of the gas is back to the left partition. As will be addressed in the next section, this “intelligent being” would be also able to “violate” the 2nd law in many other different ways, shedding a light upon why the demon intrigued scientists during more than 150 years.

2.2 The “birth” of the demon

The first ever mention to the notorious thought experiment which culminates in the “violation” of the 2nd law of thermodynamics, later known as Maxwell’s demon, took place in a letter from J. C. Maxwell to P. G. Tait, written in December of 1867. (13) While discussing with his lifelong friend developments in the field of thermodynamics, Maxwell suggests that an “intelligent being” could act as to “violate” the 2nd law, in his own words, “to pick a hole in the 2nd law.” As described by himself (14):

“Now let A and B be two vessels divided by a diaphragm [...] and let them contain elastic molecules [...] let those in A have the greatest energy of motion. [...] I have shown that there will be velocities of all magnitudes in A and the same in B, only the sum of the squares of the velocities is greater in A than in B. [...] Now conceive a finite being who knows the paths and velocities of all the molecules by simple inspection but who can do no work, except to open and close a hole in the diaphragm [...] Let him first observe the molecules in A and when he sees one coming the square of whose velocity is less than the mean sq. vel. of the molecules in B let him open the hole and let it go into B. Next let him watch for a molecule of B, the square of whose velocity is greater than the mean sq. vel. in A, and when it comes to the hole let him draw the slide and let it go into A, keeping the slide shut for all other molecules. [...] the energy in A is increased and that in B diminished, that is, the hot system has got hotter and the cold colder and yet no work has been done, only the intelligence of a very observant and neat-fingered being has been employed.” (15, 16)

It is relevant to note that one of the important pillars for the development of Maxwell’s idea is his own major contribution to the kinetic theory of gases, coined later as the Maxwell’s-Boltzmann distribution. It implies that, although the gas is in thermal equilibrium, the velocities of its constituent molecules are not equal. At that time, statistical mechanics was a field at the beginning of its development, such that part of the scientific community was still skeptical about it and its implications to thermodynamics, which may have motivated Maxwell to develop his thought experiment. (13, 17) Later in December of 1870, Maxwell describes again his idea in a more concise way, in a letter to J. W. Strutt, Lord Rayleigh. In this occasion he also addresses more details on the characteristics that the “being” must own in order to act as desired, and even questions how much “intelligent” it must be. As follows:

“Put such a gas in a vessel with two compartments and make a small hole [...] Provide a lid or stopper for this hole and appoint a doorkeeper very intelligent and exceedingly quick, with microscopic eyes, but still an essentially finite being. Whenever he sees a

molecule of great velocity coming against the door from A into B he is to let it through [...] He is also to let slow molecules pass from B to A but not fast ones [...] Of course he must be quick, for the molecules are continually changing both their courses and their velocities. [...] In this way the temperature of B may be raised and that of A lowered without any expenditure of work, buy only by the intelligent action of a mere guiding agent [...] I do not see why even intelligence might not be dispensed with and the thing made self-acting.” (18)

The public debut of the “intelligent being” occurred in 1871, discussed in a section named *Limitation of the second law of thermodynamics* of Maxwell’s book, *Theory of heat*. (19) It is clear that with his thought experiment Maxwell expected to emphasize the statistical nature of the 2nd law, that is, when there is full access to the dynamics of each constituent of matter, situations where the 2nd law is no longer satisfied could be conceived. As discussed by him:

“One of the best established facts in thermodynamics is that it is impossible in a system enclosed in an envelope which permits neither change of volume nor passage of heat, and in which both the temperature and the pressure are everywhere the same, to produce any inequality of temperature or of pressure without the expenditure of work. This is the second law of thermodynamics, and it is undoubtedly true as long as we can deal with bodies only in mass, and have no power of perceiving or handling the separate molecules of which they are made up. But if we conceive a being whose faculties are so sharpened that he can follow every molecule in its course, such a being, whose attributes are still as essentially finite as our own, would be able to do what is at present impossible to us.” (19)

Thus, from Maxwell’s original descriptions, his thought experiment can be portrayed as follows: consider a container full of gas initially at thermal equilibrium and with a partition inserted on its middle, dividing the gas in two halves, referred as A (left side) and B (right side). Assume that there is a small gate in the partition that can be opened and closed, without the requirement of doing work, and that there is an “intelligent being” controlling this opening mechanism. And even more, this “being” is also able to detect the position and velocities of all particles, meaning that he has access to the full dynamics of the gas. Therefore, the “being” is able to make use of the information he posses on the dynamics, in order to decide if the gate must be opened or closed, and consequently, if the particles will go from one side of the partition to the other, Fig. 2.2.1.

As is known, the velocities of the particles are not equal and satisfy a probability distribution, the Maxwell’s-Boltzmann distribution, such that the mean square velocity of the particles is related to the temperature of the gas. So, when the “being” detects a particle in half A going in the direction of B, with a velocity smaller than the mean square velocity of the gas, he opens the gate, allowing

Figure 2.2.1 – Portray of Maxwell's thought experiment. There is a container full of gas initially at a thermal equilibrium state with a partition inserted on its middle. There is also a small gate in the partition that can be opened and closed by the demon, without the requirement of doing work. The particles of the gas are the colored circles and the arrows represent their velocities. Particles with velocities higher (smaller) than the mean square velocity of the gas are colored with different shades of red (blue).

Source: By the author

the particle to pass through it and going to half B. However, if the velocity of the particle is higher than the mean square velocity, he does not open the gate, and the particle remains in A. For the other half he does the exact opposite: when a particle in half B is detected going in the direction of A, the gate is only opened if the velocity of the particle is higher than the mean square velocity of the gas. Therefore the “being” is sorting faster particles to the half A and slower particles to half B, as represented in Fig. 2.2.2. It is important to stress that no work is done in this sorting process, this “being” just enables some particles, that would naturally collide with the partition, to maintain their trajectories and go to the other side of the container.

This sorting process is repeated several times, actually it must be ideally repeated an infinite amount of times in order to the two different halves of the gas to achieve thermal equilibrium, each one with a different temperature. So the gas initially at temperature T will be turned into two gases of different temperatures, with the gas at half A having a higher temperature than the gas at half B, Fig. 2.2.3. This constitutes a serious “violation” of the 2nd law of thermodynamics, as a difference in temperature is created in a system initially at thermal equilibrium, without any work done. Or in other words, heat was transferred from a cold gas to a hot gas, without an external agent performing work, in a direct “violation” to the Clausius statement of the 2nd law. Finally, this “violation” can be also stated in terms of entropy, although Maxwell's himself did not make use of the concept of entropy when describing the action of his “being.” (13) This is, the entropy of the initial gas at temperature T is higher than the sum of the entropies of the two gases when at different temperatures, and so the action of the “being” was responsible for diminishing the entropy of the system without doing any work, which is not allowed by the 2nd law.

Figure 2.2.2 – Representation of the working of the demon, that is able to define which particles should pass through the gate. As the demon has full access to the dynamics of the gas, that is, the position and velocities of all its particles, it executes a sorting process. The demon opens or closes the gate in the middle of the partition depending on whether he wants the particle that is approaching to go to the other half of the container or to stay in the same half. Particles with velocities higher than the mean square velocity of the gas, represented in shades of red, are allowed to go from half B to half A, or stay in half A. Particles with velocities smaller than the mean square velocity of the gas, represented in shades of blue, are allowed to go from half A to half B, or stay in half B.

Source: By the author

Figure 2.2.3 – Result of the action of the demon, after the completion of an infinite amount of sorting processes. The two different halves of the gas will reach thermal equilibrium each one with a different temperature. Half A, which received the particles with higher velocities (shades of red), will reach thermal equilibrium with a higher temperature than half B, which received the particles with smaller velocities (shades of blue). So the demon has apparently “violated” Clausius statement of the 2nd law.

Source: By the author

It is worth mentioning that the folkloric denomination, “Maxwell’s demon,” attributed to the “intelligent being” acting in Maxwell’s thought experiment, was given by Lord Kelvin, in 1874. The original idea was not to address the “being” as a personification of malignity, but to emphasize its “supernatural” power of “*observing and influencing individual molecules of matter*,” as described by Thomson himself. (13) Over time, Maxwell adopted the use of the term demon and broadened its definition, including not just the ones capable of creating a difference in temperature but also demons that create a difference in pressure. This can be clearly seen in the following passage, extracted from an undated letter to Tait and named *Concerning demons*:

“Is the production of an inequality of temperature their only occupation? No, for less intelligent demons can produce a difference in pressure as well as temperature by merely allowing all particles going in one direction while stopping all those going the other way. This reduces the demon to a valve.” (15)

Unfortunately, it is not possible to know if Maxwell’s considered his demon to be a serious threat to the 2nd law, requiring a proper “exorcism.” However, in the hand of the next generations of scientists, the demon created a life of its own. Considerable effort was put to further investigate and to develop the concepts underlying the working of the demon, including considerations about its intelligence, its means of detecting information about the individual dynamics of the particles, and whether it really constitutes a “violation” of the 2nd law.

One example of a non-intelligent demon is Smoluchowski’s trap door, devised in 1912. (13) The idea was that a one-way valve, inserted at the middle of a container with gas prepared initially

Figure 2.2.4 – Representation of Smoluchowski’s trap door, example of a pressure demon. The role of a non-intelligent demon is assumed by a valve inserted in the middle of a container with gas initially at equilibrium. The working of the valve is such that it only opens to one side. That is, when a particle at the left side of the container collides with the valve, it will open and let the particle go to the right side of the container. However, when a particle from the right side collides, the valve does not open and the particle remains at the right side of the container. That is, the valve would be able to trap all the particles to half of the initial volume of the gas without doing any work. However, this is actually not possible, as because of thermal fluctuations the valve will eventually let particles trapped at the right side to scape to the left side. And so, the 2nd, is not violated.

Source: NORTON. (21)

at an equilibrium state, would undertake the role of a demon and create a pressure difference on the gas. When a particle at the left side of the container collides with the valve, it will open and let the particle go to the right side of the container. And when a particle from the right side collides with the valve, it will not open and the particle remains at the right side of the container, see Fig. 2.2.4. This non-intelligent demon would be able to trap all the particles of the gas on the right side of the container, reducing the gas to half of its initial volume without the expenditure of work. However, as pointed by Smoluchowski himself, this is actually not possible, as because of thermal fluctuations the valve will eventually let particles trapped at the right side to scape back to the left side. That is, the Brownian movement from the particles colliding against the valve, would make it heat up and begin to vibrate, ceasing to work as a one-way valve. And so, this valve would not actually work as desired, showing that this type of non-intelligent mechanical demon cannot operate ^{vi}.

And in 1929, one major development on the understanding of the demon took place when Szilard’s published his iconic work *On the decrease of entropy in a thermodynamic system by the intervention of intelligent beings*. (22) In this paper, Szilard describes an engine operated by an “intelligent man,” acting in an one molecule gas, that is able to “violate” the 2nd law by extracting heat from a bath and totally converting it into work in a cycle. The importance of this model relies on its simplicity, as it is no longer necessary to deal with the complex dynamics of a multi-particle

^{vi} Later in 1963, Feynman further elaborated Smoluchowski’s idea in what is now known as Feynman ratchet or Brownian ratchet. (20)

gas as in Maxwell's original thought experiment, and the role of the demon is reduced to a binary measurement and decision making. As described by Szilard:

“A standing hollow cylinder, closed at both ends, can be separated into two possibly unequal sections [...] by inserting a partition from the side at an arbitrarily fixed height. This partition forms a piston that can be moved up and down in the cylinder. An infinitely large heat reservoir of a given temperature T insures that any gas present in the cylinder undergoes isothermal expansion as the piston moves. This gas shall consist of a single molecule [...] Imagine, specifically, a man who at a given time inserts the piston into the cylinder and somehow notes whether the molecule is caught in the upper or lower part [...] The man moves the piston up or down depending on whether the molecule is trapped in the upper or lower half of the piston. [...] this motion may be caused by a weight, that is to be raised, through a mechanism that transmits the force from the piston to the weight [...] It is clear that in this manner energy is constantly gained at the expense of heat.” (22)

Based on Szilard's original work, his idea can be simplified and explained as follows, see Fig. 2.2.5. Consider a hypothetical one particle gas trapped in a container, of volume V , in contact with a thermal bath at temperature T . A partition, for now fixed, is inserted in the middle of the container, and the particle becomes trapped in either one of the sides of the container, left or right. The “intelligent being,” the demon, is able to measure the position of the particle and also couple a system of weight and pulley to one of the sides of the partition without doing any work. Then, the partition is allowed to move. Note that if the system of weight and pulley is coupled to the same side where the particle is trapped, the one particle gas will expand, absorbing heat from the bath and doing work while lifting the weight in an isothermal expansion^{vii}. However, if the system of weight and pulley is coupled to the opposite side as where the particle is trapped, this will not happen and no work can be extracted. So, the role of the demon is precisely to detect, after the insertion of the partition, the side where the particle is trapped and couple the system of weight and pulley to this same side, in order to guarantee that work, W , will be extracted and heat, Q , will be absorbed from the bath during the process. This is, the demon is responsible for carrying out a binary decision, where the result of its measurement, left or right, defines which operation should be applied to the system. At the end of the process the partition is removed, returning the gas to its initial state. Since the expansion is isothermal and the gas is considered ideal, one finds that^{viii}:

^{vii} Ideally, the weight must be continuously changed in such a way that the force it applies in the partition during the expansion equals the force resulting of the pressure of the one molecule gas. This guarantees that the process is quasistatic and reversible.

^{viii} For an ideal gas the internal energy depends only of the temperature, so in an isothermal process as the one described, it will assume a constant value.

$$Q = W = \int_{V/2}^V P dV = Nk_B T \int_{V/2}^V \frac{1}{V} dV = k_B T \ln(2) \quad (2.2.1)$$

So, the working of this engine operated by the demon is such that heat is extracted from a bath and fully converted into useful work, and no other change is made to the environment, as the state of the gas is the same as in the beginning, which presents a serious “violation” to the Kelvin statement of the 2nd law. Or also, it can be seen that the total entropy variation of the system is negative and equal to $-k_B \ln(2)$, as heat has been absorbed from the bath, representing a “violation” of the 2nd law, as the total entropy of an isolated system must not decrease. That is, Szilard’s engine acts as a perpetual-motion machine of the second kind, that does not exist in nature.

Szilard himself proposed a solution to this apparent paradox, arguing that in order to satisfy the 2nd law, an amount equal to at least $k_B \ln(2)$ of entropy should be created during the measurement procedure performed by the demon. He models that the measuring process, that is, the gathering of information, is accomplished by the process the coupling the system with a memory. However, in his work is not clear if the entropic cost is associated with measuring, remembering or forgetting the information collected by the demon. Although currently this is not considered as the complete solution to the paradox, Szilard’s idea led to the establishment of the important link between information and thermodynamics and also to the use of the concept of memory, that would later play a special role in the proper “exorcism” of the demon.

There were some other attempts to solve the “violation” created by the demon, and L. Brillouin, later in 1951, proposed that the measuring process is actually the one responsible for generating an entropic increase in the system that compensates the diminish in entropy of the gas. He argued that the demon must make use of light signals in order to detect the particles in the gas, as in an enclosure at constant temperature the radiation is that of a blackbody, and the demon cannot see the particles. So, there should be an external source lighting the gas. A particle is detected when at least one quantum of energy is scattered by it and then absorbed by the “eye” of the demon, increasing the entropy of the demon. (23) This reasoning was accepted as the correct one during some time, until the real “exorcism” was presented by C. Bennett in 1982, as discussed in the following Section.

Figure 2.2.5 – Representation of the steps of operation of a Szilard's engine. A partition is released in the middle of a container in which there is an idealized one particle gas, represented as a pink circle. The demon measures in which side of the partition the particle is localized, left or right. Without doing work the demon couples a system of weight and pulley to the same side of the partition as in which the particle of the gas is. Then the one particle gas is allowed to expand, absorbing heat, Q , from the bath and converting it into work, W , during an isothermal process. At the end, the gas is returned to its same initial state, and apparently the Kelvin statement of the 2nd law is “violated”.

Source: By the author

2.3 The “exorcism” of the demon

The proper “exorcism” of the demon is accomplished when the famous Landauer’s principle, dated of 1961, was applied by C. Bennett to understand the process of information discard undergone by the memory of the demon. The key point is that in all past analysis, no change was attributed to the demon itself, implicitly assuming that its measuring process could be achieved without resulting in any further entropic change. And this is no truth, as the information gathered by the demon must be physically stored in a memory and later erased, in order to restore the demon to its initial state, and this process of discarding information is necessarily associated with an increase in entropy. The road that lead to the construction of this solution to the conundrum created by Maxwell’s demon was long and arduous, and here a glimpse of this process is presented.

As mentioned before, Szilard, back in 1929, already identified the three central issues essential to solve the puzzle of Maxwell’s demon: information, measurement and memory. (13) Later in 1932, J. von Neumann in his book *Mathematical foundations of quantum mechanics* (24), while arguing that the insertion of the partition in Szilard’s engine does not affect its ensemble entropy, already discussed the fact that entropy decrease was associated with the demon’s knowledge on the system:

“[...] at the end of the process, the molecule is again in the volume V , but we no longer know whether it is on the left or right [...] Hence there is a compensating entropy decrease of $k_B \ln(2)$ (in the reservoir). That is, we have exchanged our knowledge for the entropy decrease of $k_B \ln(2)$.” (13)

Unfortunately, there is no mention to the essential final step of discarding the information collected by the demon. However, in 1970, independently of Landauer’s work and prior to Bennett’s publications on the demon, O. Penrose addressed in his book, *Foundations of statistical mechanics* (25), the importance of the erasure of the demon’s memory, that would be responsible for sending entropy to the environment. He argues that in the case of a perpetual motion machine, responsible for extracting work from thermal fluctuations, in order to complete its cycle, it must suffer a reset process to its initial state. And so what he calls as the latent contribution to the entropy, resulting from the observational states necessary for the machine to actually perform work and cause the reduction of entropy, will be further manifested as entropy on the environment during this reset process:

“[...] The large number of observational states that the Maxwell demon must have in order to make significant entropy reductions possible may be thought of as a large memory capacity in which the demon stores the information [...] As soon as the demon’s memory is completely filled [...] he can achieve no further reduction of the

Boltzmann entropy [...] for the erasure being a setting process, itself increases the entropy by an amount at least as great as the entropy decrease made possible by the newly available memory capacity.” (25)

Penrose's analysis is not as complete as the work later accomplished by Bennett in understanding the working of the demon, yet it is clearly an important treatment on memory erasure, achieving in a slightly different context the same conclusions stated in Landauer's principle. Unfortunately, this results went largely unnoticed by the scientific community studying Maxwell's demon and its related topics. (13)

So back in 1961, R. Landauer published his seminal work, *Irreversibility and heat generation in the computing process* (26), where he states that computing machines will inevitably perform logically irreversible operations, necessarily associated with physical irreversibility, which in turn requires a minimal amount of heat generation in order to be accomplished. Landauer's ideas established the concept of a minimum theoretical limit of energy consumption during the computation process, and as written by himself:

“[...] we can show, or at least very strongly suggest, that information processing is inevitably accompanied by a certain minimum amount of heat generation. Computing, like all processes proceeding at a finite rate, must involve some dissipation. Our arguments, however, are more basic than this, and show that there is a minimum heat generation, independently of the rate of the process.” (26)

The argument constructed in the article is that in order to label a machine as logically reversible, i.e., from the output of the operation it is possible to obtain unequivocally its input, all its intermediary steps must be also reversible. For that, additional information must be saved, cluttering up the machine's memory with unnecessary information during a long program. An example of a logically irreversible process is precisely the erasure of information. Based on the demand that information must be stored in a physical system^{ix}, Landauer introduces a model where the bits used to encode information, 0 and 1, are represented as the position of a particle in a bistable potential well. When the coordinate for the position of the particle, x , is smaller (bigger) than 0 the bit 0 (1) is encoded in the system, see Fig. 2.3.1. So, the erasure process is defined as restoring the state of the physical bit to a predefined value, regardless of its initial value, as an example, the action restore to 1. Of course, if the initial state is known, different protocols can be applied when erasing the bit, guaranteeing that the process is completed without the expenditure of energy. That is, if the particle already is in state 1, it will be maintained in this state. If it is in state 0, a force can be applied pushing it over the barrier, and then after it has passed the maximum, a retarding force is applied and the particle finishes the process in the right side of the potential with no excess kinetic energy. However

^{ix} Landauer later coined that “Information is physical” in his work of the same name. (27)

this is not a genuine erasure process, as information on the initial state related to which protocol was used, is still retained. And as the laws of mechanics are deterministic, it is not possible to construct a single protocol, composed of a force varying in time applied to a conservative system, that will always restore the particle to state 1 regardless of its initial state. (13, 26) This reasoning implies that in order to erase information, the potential well must be lossy, such that the dynamics becomes dissipative and there will be an intrinsic energy dissipation associated with the erasure process. Landauer further elaborates his idea, considering a statistical ensemble of bits initially at thermal equilibrium and that undergoes the erasure process, therefore being all reset to the same state. As both states have the same energy, they are equally distributed initially and erasing them will diminish the entropy of the system by a term equal to $k_B \ln(2)$. However, as stated by the 2nd law of thermodynamics, the entropy of a closed system must not decrease, and this entropy will appear elsewhere as heating effect. So, it is argued that the irreversible process of erasure will be necessarily accompanied by an entropy increase, and this is known as Landauer’s principle.

Figure 2.3.1 – Representation of the physical model encoding one bit of information considered by Landauer. There is a particle in a bistable potential well, $U(x)$, and if the coordinate for the position of the particle is such that $x < 0$ ($x > 0$) the bit 0 (1) is encoded in the physical system.

Source: By the author

Influenced by Landauer’s work, Bennett devoted himself to investigate if general-purpose computation could actually be performed in a logically reversible apparatus without the downfalls pointed by Landauer on always saving the excessive information on the intermediate states. In his article *Logical reversibility of computation* (28), dated from 1973, Bennett conceived a computation model where all steps are reversible and the process of execution is such that when a given segment of operations is taken, the intermediate result is printed and the machine undergoes the reverse of its operations, in such a way to use the extra information in order to reverse the process, restoring the state of the memory as the same as before the application of the initial steps, however without the need to delete any information. At the end of this process, the final output of the total computation is obtained together with the initial input and intermediate outputs only

of the segments, and the memory of the apparatus is restored to its initial state. Implying so that a computation without the minimum dissipation of energy, required by Landauer's principle, can be, at least theoretically achieved. This idea latter inspired Bennett to reinterpret the solution to Maxwell's demon, arguing that the solution to its paradox actually stands in the entropic cost of erasing the information collected by the demon, and not on the energetic cost of measurement, as accepted so far. As stated by him in his 1982 famous article, *The thermodynamics of computation - a review*:

"[...] the essential irreversible act, which prevents the demon from violating the second law, is not the measurement itself but rather the subsequent restoration of the measuring apparatus to a standard state [...] This forgetting of a previous logical state [...] entails a many-to-one mapping of the demon physical state, which cannot be accomplished without a corresponding entropy increase elsewhere." (29)

He argues that in the case of Szilard's engine the demon acts in an analogous way as a computation apparatus, measuring in which side of the partition the particle is and storing this information in the memory, 0 if it is at the left and 1 if it is at the right. And, as reasoned by Bennett, this process can be achieved in a reversible way, without any dissipation. Later the demon continues its operation depending on what is stored in its memory, and is able to extract work. However, because of the storing of information necessary to the accomplishment of the operation, the final state of the demon's memory is not the same as the initial state. So, in order to the Szilard's engine to really complete a cycle, the memory of the demon must be erased and restored to its initial state. As stated by Landauer's principle, this final step of erasing one bit of information will necessarily generate an energetic dissipation and an entropy increase to the system at least equal to $k_B \ln(2)$. Thus the entropy generation associated with the irreversible process of erasure compensates exactly the energy decrease caused by the demon, and actually there is no "violation" of the 2nd law of thermodynamics.

Applying also this reasoning to Maxwell's original thought experiment, the demon must store all the information of the particles velocities when they are getting closer to the partition gate, and then operate, letting or not the particle go through it. However, the process of measuring and then storing this into the memory undergoes until the system achieves thermal equilibrium again, i.e., it is repeated an infinite amount of times. But the memory itself is a physical object and there does not exist in nature a memory with an infinite amount of physical storage. Thus, this information must be later erased, in order to the demon to keep its sorting processes and continue to use its memory. And so, this necessary erasing process will be accomplished by coupling the demon, or at least, its memory to a bath, causing the dissipation of heat and consequently the increase of entropy. In this way, Bennett's arguments saves the 2nd law from being violated by this "intelligent being."

However, there were criticisms to Landauer’s principle and consequently to the solution of the Maxwell’s demon paradox presented by Bennett, precisely by pointing that the argument leading to the development of Landauer’s principle was not rigorous enough. It was argued that the whole line of thought is circular, as the 2nd law is applied to create a solution to a problem where the 2nd law itself is apparently being violated. Later in 1995, K. Shizume presented a proof of Landauer’s principle. (30) Using the Langevin equation describing the motion of a Brownian particle in a bistable potential well, he showed that the erasure of one bit of information will lead to a minimum dissipation of heat, equal to $k_B \ln(2)$, in a constant temperature thermal bath. In addition, without evoking the 2nd law in 2000, B. Piechocinska presented an even more complete proof, including both the classical and quantum case, supporting that Landauer’s principle is a concept of general validity in nature. (31) In her analysis for the classical continuous case, the same physical model of a particle, of mass m , in a bistable potential well, $U(x)$, in contact with a bath at temperature T , is used to represent a bit, see Fig. 2.3.1. The erasure protocol is such that regardless the state of the particle at the initial time t_i it will end in the state representing bit 1 at the final time t_f . The hamiltonian of the total system, particle plus bath, is given by:

$$H_T(x, p, \vec{r}_B, \vec{p}_B) = \overbrace{H(x, p)}^{\text{Particle}} + \overbrace{H_B(\vec{r}_B, \vec{p}_B)}^{\text{Bath}} + \overbrace{H_I(x, p, \vec{r}_B, \vec{p}_B)}^{\text{Interaction}} \quad (2.3.1)$$

where the position and momentum of the particle are respectively, x and p and the degrees of freedom associated with the bath are represented by $\vec{r}_B$ and $\vec{p}_B$. Also, the hamiltonian of the particle is simply $H(x, p) = \frac{p^2}{2m} + U(x)$. Therefore, in the case of a weak interaction, the canonical ensemble provides that the initial distribution functions for the particle, $\rho_i(x(t_i), p(t_i))$, and the bath, $\rho_{B_i}(\vec{r}_B(t_i), \vec{p}_B(t_i))$, are equal to:

$$\rho_i(x(t_i), p(t_i)) = \frac{1}{Z} e^{-\beta H(x(t_i), p(t_i))} \quad \text{and} \quad \rho_{B_i}(\vec{r}_B(t_i), \vec{p}_B(t_i)) = \frac{1}{Z_B} e^{-\beta H_B(\vec{r}_B(t_i), \vec{p}_B(t_i))} \quad (2.3.2)$$

where the partition function for the particle is $Z = \iint dx dp e^{-\beta H(x, p)}$ and analogously for the bath $Z_B = \iint d\vec{r}_B d\vec{p}_B e^{-\beta H_B(\vec{r}_B, \vec{p}_B)}$. At the end of the erasure process, as the particle will be necessarily at state 1, the probabilities distributions are:

$$\rho_f(x(t_f), p(t_f)) = \begin{cases} 0 & , x < 0 \\ \frac{1}{Z/2} e^{-\beta H(x(t_f), p(t_f))} & , x > 0 \end{cases} \quad \text{and} \quad \rho_{B_f}(\vec{r}_B(t_f), \vec{p}_B(t_f)) = \frac{1}{Z_B} e^{-\beta H_B(\vec{r}_B(t_f), \vec{p}_B(t_f))} \quad (2.3.3)$$

where the partition function for the particle is half as initially, because the potential is symmetrical

and the particle is confined to half of its initial space. And for the bath the partition function is unchanged. To describe the temporal evolution of all degrees of freedom of the total system, the notation $\zeta(t) \equiv (x(t), p(t), \vec{r}_B(t), \vec{p}_B(t))$ is adopted, defining the state of the particle and the bath at any time t . So, during the execution of the protocol to erase the memory, there is a deterministic evolution from state $\zeta_i = \zeta(t_i)$ to $\zeta_f = \zeta(t_f)$.

And then a new variable, $\Gamma(\zeta_i, \zeta_f)$, which is a function of the final and initial probabilities densities of the particle and the bath, is defined as:

$$\Gamma(\zeta_i, \zeta_f) = -\ln[\rho_f(x(t_f), p(t_f))] + \ln[\rho_i(x(t_i), p(t_i))] + \beta Q \quad (2.3.4)$$

where $Q \equiv H_B(\vec{r}_B(t_f), \vec{p}_B(t_f)) - H_B(\vec{r}_B(t_i), \vec{p}_B(t_i))$ is equal to the variation of the hamiltonian of the bath, i.e., is the heat dissipated to the bath during the process. So the average, on the ensemble of all possible initial configurations, of the variable $e^{-\Gamma}$ is calculated, such that:

$$\begin{aligned} \langle e^{-\Gamma} \rangle &= \int d\zeta_i \rho_i(x(t_i), p(t_i)) \rho_{B_i}(\vec{r}_B(t_i), \vec{p}_B(t_i)) e^{-\Gamma(\zeta_i, \zeta_f)} \\ &= \frac{1}{Z_B} \int d\zeta_i \rho_i(x(t_i), p(t_i)) \frac{e^{-\beta H_B(\vec{r}_B(t_f), \vec{p}_B(t_f))} \rho_f(x(t_f), p(t_f))}{\rho_i(x(t_i), p(t_i)) e^{-\beta H_B(\vec{r}_B(t_i), \vec{p}_B(t_i))}} \\ &= \int d\zeta_f \rho_f(x(t_f), p(t_f)) \rho_{B_f}(\vec{r}_B(t_f), \vec{p}_B(t_f)) = 1 \end{aligned} \quad (2.3.5)$$

in which a change in integration variables from ζ_i para ζ_f is made, where the Jacobian of this transformation is equal to 1, as the evolution of the system is hamiltonian. So, $\ln \langle e^{-\Gamma} \rangle = 0$ and using Jensen's inequality^x it is possible to write that:

$$\begin{aligned} -\langle \Gamma \rangle &\leq 0 \\ \beta \langle Q \rangle &\geq \langle \ln[\rho_f(x(t_f), p(t_f))] \rangle - \langle \ln[\rho_i(x(t_i), p(t_i))] \rangle \\ \beta \langle Q \rangle &\geq \iint dx(t_f) dp(t_f) 2\alpha(x(t_f), p(t_f)) \ln(2\alpha(x(t_f), p(t_f))) \\ &\quad - \iint dx(t_i) dp(t_i) \alpha(x(t_i), p(t_i)) \ln(\alpha(x(t_i), p(t_i))) \end{aligned} \quad (2.3.6)$$

in which it was defined that $\alpha(x, p) = e^{-\beta H(x, p)}/Z$. The region of integration associated with the variable $x(t_f)$ is half of the region of integration of variable $x(t_i)$. And also the potential function $U(x)$ is symmetric, implying that $\alpha(x, p) = \alpha(-x, p)$. So the expression can be simplified as:

^x Jensen's inequality states that for any convex function, $f(x)$, and random variable x : $f(\langle x \rangle) \leq \langle f(x) \rangle$. So, $e^{\langle x \rangle} \leq \langle e^x \rangle$ and applying the logarithmic function, which is convex, it is obtained that $\langle x \rangle \leq \ln \langle e^x \rangle$.

$$\begin{aligned}
\beta \langle Q \rangle &\geq \iint dx(t_i) dp(t_i) \alpha(x(t_i), p(t_i)) [\ln(2\alpha(x(t_i), p(t_i))) - \ln(\alpha(x(t_i), p(t_i)))] \\
\beta \langle Q \rangle &\geq \underbrace{\iint dx(t_i) dp(t_i) \alpha(x(t_i), p(t_i)) \ln(2)}_1 \\
\langle Q \rangle &\geq k_B T \ln(2)
\end{aligned} \tag{2.3.7}$$

in such a way that exactly Landauer's principle is obtained. That is, there is a minimum average heat dissipated to the bath during the erase of one bit of information, and it is equal to exactly $k_B T \ln(2)$ ^{xi}.

And the discussion of the proof of Landauer's principle for the quantum case is left to the following Section 2.4, in which the later works extending Maxwell's demon to the domain of quantum mechanics are addressed.

2.4 Maxwell's demon in the quantum realm

Maxwell's thought experiment was imagined at a time where statistical physics was still under development, classical mechanics reigned absolute and the atomic theory was not a consensus among the scientific community. All the later development on the aspects of the demon and the solution to its paradox occurred concurrently to the scientific revolution that gave rise to quantum mechanics. And in the mid 1980's, the nuances that may emerge when the demon enters the quantum realm started to be intensely investigated.

In 1984, W. Zurek examined a quantum mechanical version of Szilard's engine. (32) He modeled the one particle gas inside the container as a particle in a square potential well, and that must be also coupled to a thermal bath of temperature T . The partition inserted at the middle of the container during the working of the engine is analogous to a narrow potential barrier, of height U and width δ . The height of the barrier can be slowly increased, corresponding to the process of inserting the partition. Also it must satisfy $U \gg k_B T$, such that the bath will not be able to create excitations of the particle above the barrier, see Fig. 2.4.1.

^{xi} It is also possible to proof Landauer's principle applying only the concept of Helmholtz free energy and the fact that the process of erasure is actually responsible for diminishing the partition function of the system to half of its initial value. Helmholtz free energy, F , is related to the total energy of the system, U , temperature, T and entropy, S such that $F = U - TS$. The process of erasure is isothermal, and so the variation of Helmholtz free energy is equal to $\Delta F = \Delta U - T \Delta S$. As $\Delta S \geq Q/T$ and it is assumed that $\Delta U = 0$, then $Q \geq \Delta F$. Helmholtz free energy is defined as being equal to $-k_B T \ln(Z)$, where Z is the partition function. As already discussed, during the erasing protocol the final partition function is equal to half of the initial partition function, such that $\Delta F = -k_B T [\ln(Z_i/2) - \ln(Z_i)] = k_B T \ln(2)$. So, it is obtained that $Q \geq k_B T \ln(2)$, which is exactly the statement of Landauer's principle

Figure 2.4.1 – Representation of Zurek's quantum Szilard's engine. In (a) the operating steps of the Szilard's engine are represented. In (b) the model for a quantum mechanical version is represented. The one particle gas is modeled as a particle inside a square well potential. The insertion of the partition is analogous to the height of a narrow potential barrier, U , being slowly increased.

Source: ZUREK. (32)

After the insertion of the potential barrier, the particle is in a quantum state $|\psi_n\rangle$, that is a superposition state of the eigenfunctions for the left and right sides of the barrier, respectively $|L_n\rangle$ and $|R_n\rangle$. And when a measurement is accomplished, the quantum state of the particle will be given by $|L_n\rangle$ or $|R_n\rangle$, if the particle is detected to be in the left or right side of the barrier. Until this detection is realized no work can be extracted, and as in Szilard's original engine, the demon is the one responsible for accomplishing this measurement process. Zurek models the demon as a two state quantum system, with eigenstates $|D_L\rangle$ and $|D_R\rangle$. The process of interaction between the demon and the particle is such that if the state of the particle is $|L_n\rangle$ ($|R_n\rangle$) the demon will be taken from a "ready to measure state" $|D_0\rangle$ to $|D_L\rangle$ ($|D_R\rangle$). Zurek's work introduces more of conceptual view to the analysis of the quantum demon, discussing the information exchange between the demon and the particle. It is relevant to note that there is a fundamental criticism that could be applied to Zurek's model: is it really possible to insert the potential barrier without the expenditure of work? It could be simply argued that the work done is really small and can be neglected. This has been analyzed recently by Alicki (33), who used more realistic models to implement the partition, showing that actually this work is not that small at all, and can not be ignored. So the pursue continues for physical models in which there is no involvement of any kind of processes that require work to be done on the system, as the absence of realization of work is

one of the fundamental characteristics of a genuine demon.

Later in 1997 S. Lloyd presented a version of a quantum demon that, differently from the one discussed by Zurek could be experimentally implemented. (34) He considered a nuclear magnetic resonance model, with particles with spin-1/2, $|\uparrow\rangle$ and $|\downarrow\rangle$, embedded in a constant magnetic field pointing to the $-\hat{z}$ direction. Such that the magnetic interaction energy is equal to $-\mu B$ (μB) when the magnetic moment of the particle, $\vec{\mu}$, and the field are parallel (antiparallel). A spin flip can be induced using a so-called π pulse, and if the spin state goes from state $|\uparrow\rangle$ to $|\downarrow\rangle$ ($|\downarrow\rangle$ to $|\uparrow\rangle$), the interaction energy with the field is decreased (increased) by $2\mu B$. If the energy is decreased (increased) a photon is emitted (absorbed) and the spin does positive (negative) work in the electromagnetic radiation field. The key aspect for this implementation is that the measurement of a particle's spin can be made by a reference spin. And so, by knowing the state of the spin, a π pulse can be sent in order to always induce spin flips that will result in work being done on the field. That is, a NMR demon can be implemented, using information on the state of a spin and trading it for thermodynamic advantage, in this case, the extraction of work. As always there is no “violation” of the 2nd law, since the spin must be restored to its initial state, which is done through the contact with a bath.

Figure 2.4.2 – Representation of the quantum physical model encoding one bit of information considered by Piechocinska. There is two level system, with eigenstates $|0\rangle$ and $|1\rangle$ and respective energies $\hbar\omega_0$ and $\hbar\omega_1$. If the system is in state $|0\rangle$ ($|1\rangle$), then the bit encoded is 0 (1). There is an external parameter, $\lambda(t)$, that controls the energy gaps between both states.

Source: By the author

So now, it is worth returning to the proof of Landauer's principle in the quantum case. Piechocinska proposes a physical model for storing information which is composed of a two level system, with eigenstates represented as $|0\rangle$ and $|1\rangle$, Fig. 2.4.2 (31). If the system is in state $|0\rangle$, the encoded bit is 0 and if it is in $|1\rangle$ the encoded bit is 1. Analogously to the classical case, the two level system must be in contact with a thermal bath of temperature T in order to be possible to realize the erasure process, characterized as the return to 1 operation. So although the fact that the dynamics of the two level system will be dissipative, the evolution of the universe, two level system plus the bath, is described by an unitary operator, $\hat{U}$. Such that the final density matrix describing the universe at

the end of the erasure process, $\hat{\rho}_f$, is given as $\hat{\rho}_f = \hat{U}\hat{\rho}_i\hat{U}^\dagger$. Also, the total hamiltonian is defined as:

$$\hat{H}_T(t) = \overbrace{\hat{H}(\lambda(t))}^{\text{Two level system}} + \overbrace{\hat{H}_B}^{\text{Bath}} + \overbrace{\hat{H}_I(\lambda(t))}^{\text{Interaction}} \quad (2.4.1)$$

where $\hat{H}(\lambda(t)) = \hbar\omega_0(\lambda(t))|0\rangle\langle 0| + \hbar\omega_1(\lambda(t))|1\rangle\langle 1|$, and the parameter $\lambda(t)$ is externally controlled and responsible for changing the energy gap between both eigenstates. Initially the parameter is such that the energy levels are degenerate $\omega_0(\lambda_i) = \omega_1(\lambda_i)$. The hamiltonian of the bath is defined as $\hat{H}_B = \sum_m \hbar\omega_m|m\rangle\langle m|$, where $|m\rangle$ are its eigenstates. As the system is in thermal equilibrium, and considering the weak coupling approximation, the initial density matrix of the total system is given as:

$$\hat{\rho}_i = \begin{pmatrix} 1/2 & 0 \\ 0 & 1/2 \end{pmatrix} \otimes \frac{1}{Z_B} e^{-\beta\hat{H}_B} \quad (2.4.2)$$

as the energies of the two level system are initially degenerated and the partition function for the bath is equal to $Z_B = \text{tr}(e^{-\beta\hat{H}_B})$. Then, the value of $\lambda(t)$ is modified, creating an energy difference between states $|0\rangle$ and $|1\rangle$, such that $\omega_0(\lambda) > \omega_1(\lambda)$. If this difference is sufficiently large, it is possible to guarantee that, at the end of the process, the probability that the two level system being found in state $|1\rangle$ will be equal to 1, that is, the memory is erased as the two level system is restored to the state representing bit 1. So, the final density matrix is given as:

$$\hat{\rho}_f = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \otimes \frac{1}{Z_B} e^{-\beta\hat{H}_B} \quad (2.4.3)$$

And note that the bath after the erasure process will be as initially in a thermal state. However, during the process the state of the bath may be altered from $|m\rangle$ to $|n\rangle$, and so there will be a heat exchange between the two level system and the bath equal to:

$$Q = \hbar(\omega_m - \omega_n) \quad (2.4.4)$$

At the end of the erasure process the parameter λ will be returned to its initial value and the system is decoupled from the bath. Defining the new variable Γ as:

$$\Gamma = \ln[P_i(l)] - \ln[P_f(k)] - \beta Q \quad (2.4.5)$$

in which $P_i(l)$ is the probability that the system is initially at state l , that is, $P_i(0) = P_i(1) = 1/2$ and $P_f(k)$ is the probability, after the erasure process, that the system is at state k , that is $P_f(0) = 0$ and $P_f(1) = 1$.

$P_f(1) = 1$. Calculating the ensemble average for the value of $e^{-\Gamma}$, composed of all the possible initial and final states of the total system, it is obtained that:

$$\begin{aligned}
 \langle e^{-\Gamma} \rangle &= \sum_{l,m} \sum_{k,n} P_i(l) \frac{1}{Z_B} e^{-\beta \hbar \omega_m} |\langle n, k | \hat{U} | l, m \rangle|^2 e^{-\Gamma} \\
 &= \sum_{l,m} \sum_{k,n} P_i(l) \frac{1}{Z_B} e^{-\beta \hbar \omega_m} |\langle n, k | \hat{U} | l, m \rangle|^2 \frac{P_f(k)}{P_i(l)} \frac{e^{-\beta \hbar \omega_n}}{e^{-\beta \hbar \omega_m}} \\
 &= \underbrace{\sum_{k,n} P_i(l) \frac{1}{Z_B} e^{-\beta \hbar \omega_n}}_1 \underbrace{\sum_{l,m} |\langle n, k | \hat{U} | l, m \rangle|^2}_1 = 1
 \end{aligned} \tag{2.4.6}$$

where it was employed the fact that the sum in all possible initial states of $|\langle n, k | \hat{U} | l, m \rangle|^2$, which gives the probability of finding the system in a final state $|k, n\rangle$ given that its initial state was $|l, m\rangle$, must be equal to 1. So, applying Jensen's inequality:

$$\begin{aligned}
 -\langle \Gamma \rangle &\leq 0 \\
 \beta \langle Q \rangle &\geq -\langle \ln[P_i(l)] \rangle + \langle \ln[P_f(k)] \rangle \\
 \beta \langle Q \rangle &\geq -\sum_{l=0,1} P_i(l) \ln[P_i(l)] + \sum_{k=0,1} P_i(k) \ln[P_i(k)] \\
 \langle Q \rangle &\geq k_B T \ln(2)
 \end{aligned} \tag{2.4.7}$$

Landauer's principle is obtained once more, that is, also in the quantum regime the process of erasure of one bit of information will dissipate in average, at least, an amount of heat equal to $k_B T \ln(2)$. Implying that exists a fundamental lower bound for the amount of heat dissipated into the environment during the erasure process.

However, the investigation on Maxwell's demon is far from finished. In the last years, the role of decoherence, measurement and entanglement in the mechanism of its quantum version have been actively investigated. Also, the typical classical constant temperature bath gave space to baths showing genuine quantum characteristics, as being entanglement with the system. Even the concepts of work and heat in the quantum regime, with the last one being fundamental for the construction of a proof of Landauer's principle, are under intense debate. And also, with the evolution of technology, the classical and quantum versions of Maxwell's demon have been implemented in various experimental platforms, ranging from photonic and electrical devices to superconducting qubits. Thus, in the following Chapter 3, these "real life" versions of the demon are discussed, with special attention attributed to implementations using electrical devices, which were the ones with

most relevance for the development of this master's research.

Chapter 3

Maxwell's demon in electrical devices

With the ultimate resolution of the paradox created by Maxwell's thought experiment, it may seem that the demon lost its charm. However, despite that the demon actually does not violate the 2nd law, it is still worth being investigated. And with the evolution of technology, the possibility of implementing Maxwell's demon using a variety of different experimental platforms became a reality.

3.1 Experimental implementations of Maxwell's demon

Even after the final “exorcism”, the demon is far from forgotten by the scientific community. As during the last decade, the evolution of technology enabling the control of nano-mesoscopic systems, led to the possibility of implementing Maxwell's demon using many different experimental platforms. Although the approaches applied in each implementation vary in a significant amount, all of them satisfy the basic principle:

The demon is responsible for obtaining information about a system and applying an appropriate feedback action such that the entropy of the system is decreased. The demon must not realize work on the system.

That is, the demon must be able to extract information and trade it for some thermodynamic advantage, as for example to enable the extraction of useful work. Recall that the entropy of the demon will increase during the process, in such a way that the 2nd law is not violated. One of the first experiments regarding Maxwell's demon (35, 36) was presented by the group of D. Leight, back in 2007. This work, *A molecular information ratchet*, (37) was based on the fact that knowing the position of a specific macrocycleⁱ in the molecule of rotaxaneⁱⁱ would allow direct light to be used to drive the system into a preferred non-equilibrium state. So, Leight's device was able to drive

ⁱ Molecules and ions containing twelve or more membered ring.

ⁱⁱ A large and complex organic molecule that was devised specially for this experiment.

a chemical system out of equilibrium, similar to the concept of the Brownian ratchet, while being powered by an external light source, which guarantees that the 2nd law is not violated. In 2010, Toyabe et al. (38) developed a version of the demon able to totally convert heat into work, by always moving particles against a staircase potential driven only by the energy of random collisions with the molecules that compose the substrate. The role of the demon in this case is played by an external agent, that by a camera detects the position of the particle and then applies a feedback action, changing the configuration of the potential and assuring that the particle will go against the potential. Later in 2011, M. Raizen suggested an implementation similar to the pressure version of the demon. (39, 40) The central idea was that external lasers were applied to a gas and were able to change the state of its particles. Then, the particles with a state different than the initial become trapped to one side of its compartment, such that at the end of the process all the gas is trapped to just one half of its initial volume and work can then be extracted. And in 2016 a *Photonic Maxwell's demon* (41) was implemented, using the called feed-forward operation, that directs brighter and dimmer pulses in different directions, to create an unbalance between two different light modes initially at equilibrium.

However, the implementations of major importance for this master's research do not require the use of complicated molecules or photons, they make use of the simplest possible particle, the electron. Back in 2014, Pekola's group (42) devised an implementation of Szilard's engine using only solid-state electronics. In this experiment, a SEB, Single-Electron Box, which is composed by two electronic islands connected by a tunnel junction take the role of the two chambers separated by a partition, as in Szilard's original work. In the electronic system, there are naturally many free electrons on the metal islands, but a single excess electron can be detected by an electrometer, the analogue to the one particle gas. So the demon is able to detect to which island an excess electron has tunneled and then apply the feedback operation. This operation consists on applying an external voltage controlling the tunneling of the electrons, in such a way that work $k_B T \ln(2)$ is induced by thermal activation.

Soon thereafter, in 2015, this same group developed an experiment entitled *On-chip Maxwell's demon as an information-powered refrigerator*. (1) Again, electronic devices were used, but in this case the demon is responsible for cooling the system with which it is interacting. This experiment became the main source of inspiration for the project developed in this master's, and so it is explained in details in the next section. Nevertheless, it is worth mentioning that differently from the first implementation, the work from 2015 presents a genuinely autonomous demon. As in this case there is no necessity of an external measurement apparatus, as the electrometer, to measure the state of the system and of an external agent to control the feedback process. So, in an autonomous demon, the measurement and its respective feedback operation are all interior to the device. In addition, in an non-autonomous demon, these processes occur externally to the device,

so that restricted investigation can be made on the exchange of information between the demons and its system.

Therefore, with the success of so many classical implementations of the demon, it was natural to expect that its quantum version would also become the target of many different experimentalists. Among the proposals, superconducting devices have achieved large success as platforms to implement demons. (43) As an example, there is the experiment conducted by Cottet et al. (44), in which a microwave cavity plays the role of a fully quantum autonomous demon. The cavity encodes information on the state of the system, a superconducting qubit, and the information is converted into work by powering up a microwave pulse by the stimulated emission of the qubit. Despite the significant advances in the area, there is still space for further investigation on the use of superconducting devices to implement quantum Maxwell's demons. For example, the advantages of a quantum demon over a classic one are still under investigation and even a quantum demon "violating" the Clausius statement of the 2nd law has yet to be implemented. And it was considering this novel context that the work described in this dissertation, and addressed in the Chapter 4, was developed.

3.2 Analysis of *On-chip Maxwell's demon as an information-powered refrigerator*

3.2.1 Description of the electronic device

During the last years, platforms for implementing Maxwell's demons using electrical devices were considered in the realm of theory (45, 46) and one successful and relevant experimental implementation was the one accomplished by the group of J. P. Pekola in 2015. (1) Their work has served as motivation for the development of the implementation using superconducting devices proposed in this dissertation, and so, a brief review of the setup and working of their experiment is here presented.

The platform used in the experiment conducted by Pekola's group is composed of a Single-Electron Transistor, SET, interacting with a SEB, Single-Electron Box. The SET is formed by a small normal metallic island connected in its left and right end to two normal metallic leads by identical tunnel junctions, such that the junctions permit electron transport by tunneling and possess a characteristic resistance R_{SET} . There are reservoirs of conduction electrons coupled to each end of the SET, and along the SET there is a potential difference equal to V , such that the island is in the middle of the gradient of potential. Also, associated with the two reservoirs are thermal baths with temperatures T_L and T_R , and whose thermal excitations provide enough energy for the electrons to tunnel through the SET. The role of the demon is realized by the SEB, which is composed by

Figure 3.2.1 – Pictorial representation of the elements and the tunneling dynamics in the experimental platform accomplished by the group of J. P. Pekola

Source: KOSKI. (1)

a normal metallic island connected to just one metallic lead by a tunnel junction, with resistance R_{SEB} , and also coupled to a reservoir of conduction electrons, with an associated thermal bath of temperature T_d . So the demon is able to detect the state of the SET and apply a feedback operation according to the information collected. In this case, because of its capacitive interaction with the SET, the demon is able to detect the number of excess electrons in the island of the SET, and trap an electron when it tunnels to the island with a positive charge or repel, with a negative charge, further electrons that would tunnel to the island when an electron leaves, as represented in Fig. 3.2.1a. It is important to note that the demon acts autonomously, with measurement and feedback operations occurring internally to the device.

The hamiltonian of both elements that compose the device, without considering the energy differences associated with the presence of the voltage bias along the SET, is given by:

$$H(n, N) = E_{\text{SET}}(n - n_g)^2 + E_{\text{SEB}}(N - N_g)^2 + 2J(n - n_g)(N - N_g) \quad (3.2.1)$$

where n and N are respectively the number of excess electrons in the island of the SET and of the SEB. Their charging energies are given by E_{SET} and E_{SEB} , while J defines the strength of the capacitive interaction between them. n_g and N_g are externally controlled charges, associated with capacitors coupled to the SET and the SEB, essential to govern the dynamics of the device. Now considering the energy differences caused by the existence of the potential bias in the SET, it is possible to state that an electron tunneling in the system in the direction (or against) the voltage will

experience an energy cost equal to $\Delta E = [H(n \pm 1, N) - H(n, N)] - eV/2$. An electron tunneling in the demon will experience only an energy cost equal to $\Delta E = [H(n, N \pm 1) - H(n, N)]$, as there is no voltage bias along the SEB. And the transition rates for these tunneling processes are given by the above expression:

$$\Gamma_{\text{SEB (SET)}} = \frac{1}{e^2 R_{\text{SEB (SET)}}} \frac{\Delta E}{e^{\Delta E/k_B T_{L/R}(T_d)} - 1} \quad (3.2.2)$$

such that is inversely proportional to the resistance of the junction through the electron is tunneling, it depends on the temperature of the bath that will provide the energy necessary to accomplish the tunneling, and where e is the elementary charge. Also, it is assumed the validity of the two level approximation for both elements, that is, the number of excess electrons in the metallic islands of the SET and the SEB is restricted to 0 or 1. Setting the interaction to its maximum by defining $n_g = N_g = 0.5$, the hamiltonian Eq. 3.2.1 can be simplified as the form below:

$$H(n, N) = \frac{1}{2} J(2n - 1)(2N - 1) \quad (3.2.3)$$

3.2.2 Structure of the energy levels of the electronic device

In order to give a clear view of the dynamics, it is worth representing all the different configurations of the system and their respective energies. Note that in the two level approximation, the system composed of the SEB and the SET, have four different configurations, where states $n = 1, N = 1$ ($n = 1, N = 0$) and $n = 0, N = 0$ ($n = 0, N = 1$) have the same energy, $J/2$ ($-J/2$), Eq. 3.2.3. However, the existence of the potential difference V breaks the degeneracy between the states, as the state with $n = 0, N = 0$ where no electron tunneled have a different energy than the state where, again, $n = 0, N = 0$ but an electron has tunneled from the left to the right reservoir of the SET. So, in order to account to this difference, two new variables are added to describe in totality the states, n_l and n_r , which represent the number of electrons in the left and right reservoir, allowing to keep track on the tunneling of electrons along the SET. Considering the need to satisfy conservation of charge in the devices, the system is fully described by ten different states as represented in Fig. 3.2.3, with its respective energy differences. For the sake of exemplification, in state ③, characterized by $n_l, n_r - 1, n = 1$ and $N = 0$, an electron has tunneled from the right reservoir of the SET to its island.

In this way, the desired operation of the device can be described as a sequence of tunneling events in the system and feedback operations of the demon that must result in an entropy decrease in the SET and necessarily also in a compensatory entropy increase in the demon. So, assuming that the initial state of the device is $n = 0$ and $N = 1$, that is, there is no excess electron in the SET

Figure 3.2.2 – Schematic representation of the operation of Pekola's proposed demon, which is responsible for extracting heat from the baths at the end of the SET. When an electron tunnels from the left reservoir to the island of the SET, heat Q_s is absorbed from the bath T_L ($1 \rightarrow 2$). Then, the demon, SEB, applies a feedback action, upon the detection of this tunneling, that is characterized by the change of its state from $N = 1$ to $N = 0$. During this process ($2 \rightarrow 3$) heat is released to bath T_d . In the sequence, the electron tunnels from the island to the right reservoir, and heat Q_s is absorbed now from the bath T_R ($3 \rightarrow 4$). For the last, the demon again undergoes a feedback action characterized now by the change of state from $N = 0$ back to $N = 1$ (reset), releasing heat to the bath T_d .

Figure 3.2.3 – Representation of the ten energy levels of the electronic device considering the energy differences caused by the existence of the voltage bias. The dynamics is started in state ⑩, where there is no excess or lack of electrons in the reservoirs, and the demon, SEB, is in the state $N = 1$. The transitions that occur in the desired process are represented in pink and dotted arrows: ② → ⑥ → ⑤ → ⑨ → ⑩. The final state is ⑩ where there is one excess electron in the right reservoir and the demon is again in the state $N = 1$. During this process, in total, heat $J - eV$ is absorbed from the baths in contact with the system, SET, and heat $2J$ is released to the bath in contact with the demon. It is assumed that $J > eV/2$.

Source: By the author

and there is one excess electron in the SEB. Then, an electron tunnels from the left to the island of the SET, absorbing heat equal to $Q_s = J - eV/2$ from the reservoir of temperature T_L , step 1 in Fig. 3.2.1b. In the sequence, the demon acts with its feedback operation, changing its state to $N = 0$, that is, an electron tunnels from the island of the SEB to its reservoir, releasing in meanwhile heat $Q_d = J$ to the reservoir of temperature T_d , step 2 in Fig. 3.2.1b. And now, the electron in the island of the SET tunnels to the right, also absorbing heat equal to $Q_s = J - eV/2$ from the reservoir of temperature T_R , step 3 in Fig. 3.2.1b. Last, the state of the SET and the SEB returns to the same as initially, with the demon taking again a feedback operation and returning to the state $N = 1$, that is an electron tunnels from the reservoir back to the island of the SEB, releasing again heat $Q_d = J$ to the reservoir, step 4 in Fig. 3.2.1b. So, in overall, heat has been adsorbed from the baths of temperatures T_L and T_R , causing a decrease in their entropy by the action of the demon, which is throughout the process collecting information on the state of the SET. However, the validity of the 2nd law is secured by the fact that heat is released to the bath in contact with the demon, implying in an overall increase of the entropy of the total system. So, it is worth mentioning that this whole process is only possible to be implemented with the presence of the third bath T_d , and the demon is continuously in contact with it, releasing heat, what would be analogous to the demon having its memory continuously deleted, which satisfy Bennett's solution to the Maxwell's demon paradox.

The above described sequence of tunneling events corresponds to the process of transition from the initial state ②, to ⑥, to ⑤, to ⑨ to ⑩ as represented in Fig. 3.2.3. And a simply phenomenological analysis of the dynamics allows the definition of conditions for the characteristics of the system, in such a way that the desired process actually occurs in an autonomous fashion in the system. It is important to mention that in this simple analysis, just single transitions will be considered, i.e. transitions between states in which either the state of the SET changes or the state of the SEB changes. As example, from state ② to ① a single transition has occurred, however from ② to ③ the transition occurred is not a single transition. So, initially the system is in state ②, and it can undergo single transitions, to states ① or ⑥. If $k_B T_d \ll J$, the bath of the demon does not have enough energy to create the excitation to state ①, and so the transition that will occur with more probability is to state ⑥. From ⑥, if the transition rate for the bath of the demon is higher than the rate for the baths in contact with the SET, that is accordingly to Eq. 3.2.2, $R_{\text{SET}} \gg R_{\text{SEB}}$ it will transition with more probability to state ⑤ than to state ⑩. And from state ⑤, if $k_B T_R \sim J - eV/2$, the system will transition to state ⑨. For the last, from state ⑨, it will transition to the state of lowest energy ⑩, and the process is completed as desired. That is, imposing conditions on the temperatures of the baths and its transitions rates it is possible to guarantee that the spontaneous dynamics of the system is as desired, and a Maxwell's demon is effectively implemented in this system of electronic devices.

This simple phenomenological approach to understand the tunneling dynamics played an es-

sential role in the development of the quantum autonomous Maxwell's demon proposed in this dissertation and that will be presented in the following Chapter [4](#).

Chapter 4

Autonomous quantum Maxwell's demon using superconducting devices

Inspired by the previous described research, in which electrical devices were used as a platform to implement Maxwell's demons, a superconducting system that acts as an autonomous quantum Maxwell's demon is presented. Differently from the existing implementations, this demon works mediating a heat flux from a cold to a hot bath. In this Chapter the components and the dynamics of this superconducting device are addressed and explained in details.

4.1 Description of the superconducting device

The center idea that guided the development of this work was to devise a system composed only of superconducting elements in which a Maxwell's demon could be experimentally implemented. The demon must be autonomous, that is, the demon itself must be part of the superconducting device considered, and so the exchange of information and feedback operation should occur internally to the device. Also, the system must possess a feature intrinsically quantum, as entanglement. And the way in which the demon should use information to take thermodynamic advantage is by creating a heat flux from a cold to a hot thermal bath, in an apparent "violation" of the Clausius statement of the 2nd law of thermodynamics. As expected, the entropy lowering effect caused by the demon is duly balanced by the increase of entropy of a third bath that is in contact with the demon throughout the whole process, see Fig. 4.1.1.

So, the superconducting system proposed in this work as a platform for the implementation of an autonomous quantum Maxwell's demon, Fig. 4.1.2, is composed of an ASCPT, Asymmetrical Single-Cooper-Pair Transistor, coupled capacitively to a device composed of two CPB's, Cooper-Pair Box, which are in an entangled state, being described by its antisymmetric and symmetric states, that couple capacitively to the ASCPT with different strengths. This device of entangled

Figure 4.1.1 – Simplified version of the action of the demon, in which information is used to obtain thermodynamic advantage by creating a heat flux from a cold to a hot bath.

Source: By the author

CPB's will be named as ECPB, acronym for Extended Cooper-Pair Box. In contact with the ECPB there is a thermal bath, of temperature T . There are also thermal baths at the left and right ends of the ASCPT, of temperatures T_l and T_r , respectively, where $T_l < T_r$. Before analyzing the dynamics of the whole system presented, a brief explanation on the characteristics of each individual superconducting element that compose it is presented and a deeper introduction to superconducting devices can be found in (47).

A Cooper-Pair Box, CPB, is a small superconducting island coupled by a Josephson junction to a superconducting reservoir. The junction itself acts as a potential barrier for the Cooper pairs, and can be physically implemented, as an example, by a thin insulator barrier. The Cooper pairs can tunnel across it, going in and out the superconducting island. The system can be described by the states characterized by the number n of Cooper pairs in excess in the superconducting island, denoted by $\{|n\rangle\}$ and denominated the charge basis. Also, a gate voltage can be added to the circuit, providing to the superconducting island an extra gate charge that acts as an external control parameter. And so, in the charge base, the hamiltonian of a CPB, $\hat{H}_{CPB}$, is given by (48):

$$\hat{H}_{CPB} = \sum_n \left[4E_C(n - n_g)^2 |n\rangle\langle n| - \frac{1}{2}E_J(|n\rangle\langle n+1| + |n+1\rangle\langle n|) \right] \quad (4.1.1)$$

where E_C denotes the charging energy, associated to the total capacitance of the superconducting island, E_J denotes the Josephson coupling energy, associated with the tunneling of the Cooper pairs through the junction and n_g corresponds to the dimensionless gate charge. In superconducting quantum computing, CPB's are known as the implementation of charge qubits, since only 2 states play a role in the dynamics, $|0\rangle$ and $|1\rangle$, corresponding respectively to the presence of 0 or 1 Cooper

Figure 4.1.2 – Representation of the superconducting device, composed of an ASCPT and of an ECPB, proposed as a platform for the implementation of a Maxwell's demon. The ASCPT is characterized as a superconducting island coupled to two Cooper pairs reservoirs by Josephson junctions. There is a potential difference through the ASCPT, battery, such that pairs at the left reservoir possess an extra eV of energy than the ones at the right reservoir. The ECPB is characterized by the two interacting CPBs, which are described by their entangled states, antisymmetric, $|A\rangle$ or symmetric, $|S\rangle$. The probabilities distributions, $|\langle x|A\rangle|^2$ and $|\langle x|S\rangle|^2$, associated with the localization of a Cooper pair in the region between $-L$ and L is different for both states. There are also externally controlled gates, providing extra charges n_g and N_g . There are baths of temperatures T_l and T_r in contact with the left and right ends of the ASCPT, respectively. And also a bath of temperature T in contact with the ECPB. The tunneling of Cooper pairs through the ASCPT is possible because of the thermal excitations provided by the baths T_l and T_r . The excitations between the states of the ECPB are also only possible because of thermal excitations, but provided from the bath T . The ASCPT and the ECPB interact capacitively and this interaction is proportional to J .

Source: By the author

pairs in excess in the island. (49) In this two level approximation the effective hamiltonian of a CPB is given below, where $\hat{\sigma}_z$ and $\hat{\sigma}_x$ are the Pauli matrices:

$$\hat{H}_{\text{effect. CPB}} = -2E_C(1 - 2n_g)\hat{\sigma}_z - \frac{1}{2}E_J\hat{\sigma}_x \quad (4.1.2)$$

As described, one of the components of the superconducting system analyzed, is an Asymmetrical Single-Cooper-Pair Transistor, ASCPT, which has the composition similar to that of a CPB. (50) The ASCPT is also characterized as a superconducting island, however it is coupled by identical Josephson junctions to two superconducting reservoirs, one at its left and the other at its right. So, the Cooper pairs can tunnel across the junctions, in and out the superconducting island, coming from or going to both of the reservoirs. The denomination “asymmetrical” refers to the existence of an externally controlled potential difference between the reservoirs, a battery. For the ASCPT considered, the gradient of electrical potential is such that the Cooper pairs localized in the reservoir at the left end of the ASCPT are in a potential equal to 0, the ones inside the ASCPT are in a potential $-V/4$ and the ones in the reservoir at the right are in a potential $-V/2$, and so there is an energy difference equal to eV between the Cooper pairs in the left and right reservoirs, as represented in Fig. 4.1.2. Also, the state of the ASCPT is defined in terms of the number of excess Cooper pairs in the island, $|n\rangle$, and as the term “single” in its name explicits, the dynamics of the transistor is such that just one Cooper pair can tunnel through the junction at a time, this is, the two level approximation is valid and the dynamics is described in terms of states $|0\rangle$ and $|1\rangle$.

And the other component of the superconducting system studied is the ECPB, composed of CPB 1 and CPB 2, see Fig. 4.1.2, which are characterized by the same charging and Josephson coupling energies. They are located next to each other in such a way that the interaction of the Cooper pairs in each of the islands gives origin to a capacitive coupling between the CPB's. In order to justify the previously mentioned fact that this device can be described by its entangled antisymmetric and symmetric states, the hamiltonian of both interacting CPB's, $\hat{H}_{2\text{CPB's}}$ is analyzed. Given the format of the hamiltonian of one CPB as described before, Eq. 4.1.1, and considering that there is no gate voltage in this case, we can simply write that for two identical interacting CPB's:

$$\begin{aligned} \hat{H}_{2\text{CPB's}} = & \sum_{n_1} \left[4E_C n_1^2 |n_1\rangle\langle n_1| - \frac{1}{2}E_J (|n_1\rangle\langle n_1+1| + |n_1+1\rangle\langle n_1|) \right] \\ & + \sum_{n_2} \left[4E_C n_2^2 |n_2\rangle\langle n_2| - \frac{1}{2}E_J (|n_2\rangle\langle n_2+1| + |n_2+1\rangle\langle n_2|) \right] \\ & + \sum_{n_1, n_2} C n_1 n_2 |n_1, n_2\rangle\langle n_2, n_1| \end{aligned} \quad (4.1.3)$$

where $\{|n_1\rangle\}$ and $\{|n_2\rangle\}$ are the charge bases associated respectively to the CPB 1 and the CPB 2.

Table 4.1 – Values of the eigenvalues for the ECPB in the case where $E_C/E_J = 100$ and $E_J/C = 10$

Eigenvectors	
1	$-0.707107 0, 1\rangle + 0.707107 1, 0\rangle = A\rangle$
2	$0.00176776 0, 0\rangle - 0.707105 0, 1\rangle - 0.707105 1, 0\rangle - 0.00176736 1, 1\rangle \simeq S\rangle$
3	$-0,999998 0, 0\rangle - 0.00125 0, 1\rangle - 0.00125 1, 0\rangle - 1.56232.10^{-6} 1, 1\rangle \simeq 0, 0\rangle$
4	$1,56197.10^{-6} 0, 0\rangle - 0,00124971 0, 1\rangle - 0,00124971 1, 0\rangle + 0,999998 1, 1\rangle \simeq 1, 1\rangle$

Source: By the author

The coupling is proportional to the constant C and to the term $n_1 n_2$, associated with the interaction between the Cooper pairs in excess in each CPB island. In the two level approximation for both CPB's we can write an effective hamiltonian, $\hat{H}_{\text{effect. 2 CPB's}}$, in the given form:

$$\hat{H}_{\text{effect. 2 CPB's}} = -2E_C \hat{\sigma}_{z_1} - \frac{1}{2}E_J \hat{\sigma}_{x_1} - 2E_C \hat{\sigma}_{z_2} - \frac{1}{2}E_J \hat{\sigma}_{x_2} + \frac{1}{4}C (\hat{1}_1 - \hat{\sigma}_{z_1}) \otimes (\hat{1}_2 - \hat{\sigma}_{z_2}) \quad (4.1.4)$$

in which the indexes 1 and 2 are associated with the operators acting respectively in the states of the CPB's 1 and 2. So, diagonalizing $\hat{H}_{\text{effect. 2 CPB's}}$ one of the solutions is the antisymmetric entangled state defined as $|A\rangle = \frac{1}{\sqrt{2}}(|1, 0\rangle - |0, 1\rangle)$. Also, in the regime in which $E_J \gg C$, the symmetric entangled state defined as $|S\rangle = \frac{1}{\sqrt{2}}(|1, 0\rangle + |0, 1\rangle)$ is approximately equal to one of the eigenstates of the device. More precisely, for the case where $E_C/E_J = 100$ and $E_J/C = 10$, the eigenstates are represented in Tab. 4.1.

So, if it is considered that the regime of operation is such that the ECPB will be restricted to states where the sum of Cooper pairs in excess in both islands is equal to 1, that is, the states $|1, 0\rangle$ and $|0, 1\rangle$, its effective hamiltonian, $\hat{H}_{\text{ECPB}}$, can be approximately written as:

$$\hat{H}_{\text{ECPB}} \approx E_A |A\rangle\langle A| + E_S |S\rangle\langle S| \quad (4.1.5)$$

where E_A and E_S are the eigenenergies associated respectively with the antisymmetric and symmetric states. And what makes the ECPB so essential for the suggested implementation is the fact that when it is coupled capacitively to the ASCPT, the antisymmetric and symmetric states interact with the excess Cooper pairs in the transistor with different intensities. This happens due to the fact that the probability distribution associated with the presence of a Cooper pair in the region at the middle of the two islands of the CPB's, where the ASCPT will be approximated, is smaller for the antisymmetric state, $|\langle x|A\rangle|^2$ than for the symmetric state, $|\langle x|S\rangle|^2$. So, as the interaction with the ASCPT is proportional to the effective charge existent in the ECPB, that is directly associated with the probability of finding a Cooper pair in the region where the ASCPT will be approximated, the

coupling will be stronger for the symmetric state than for the antisymmetric state. This property is easily seen in Fig. 4.1.2, where the wave functions $\langle x|0,1\rangle$ and $\langle x|1,0\rangle$ are taken as gaussians centered in the middle of each CPB's island, and the respective probabilities distributions associated with the antisymmetric and symmetric states are numerically calculated and represented in scale, as a parameter of comparison.

Thus at this point, the joint operation of the superconducting system can be introduced. So, the system, as mentioned anteriorly, is composed of an ASCPT coupled to the ECPB. It is important to notice that, as represented in Fig. 4.1.2, there are gate charges, n_g and N_g , providing an external control for the effective charge contained in the island of the ASCPT and the ECPB, respectively. Based on the above discussions of the characteristics of both superconducting elements and the nature of the interaction between them, the hamiltonian of the system, defined as $\hat{H}_{\text{ASCPT+ECPB}}$, can be written as:

$$\begin{aligned} \hat{H}_{\text{ASCPT+ECPB}} = & \sum_n E_{\text{ASCPT}}(n - n_g)^2 |n\rangle\langle n| + (E_S |S\rangle\langle S| + E_A |A\rangle\langle A|) \\ & + J \left[\sum_n (n - n_g) |n\rangle\langle n| \right] [C_S |S\rangle\langle S| + C_A |A\rangle\langle A| - N_g] \end{aligned} \quad (4.1.6)$$

The first term is referent to the energy of the Cooper pairs in the island of the ASCPT, being analogous to the first term of Eq. 4.1.1, where E_{ASCPT} is the charging energy associated with the ASCPT. The second term is the hamiltonian for the ECPB, Eq. 4.1.5 and the third one is the interaction, that has its strength controlled by the parameter J . As described, the interaction between both elements is of a capacitive nature, depending on the effective excess charge on them. The dimensionless charge contained in the island of the ASCPT is given by $\sum_n (n - n_g) |n\rangle\langle n|$ and the effective dimensionless charge in the ECPB is represented by $C_S |S\rangle\langle S| + C_A |A\rangle\langle A| - N_g$. The terms C_A and C_S account for the difference of coupling for the antisymmetric and symmetric states, as described anteriorly. As represented in Fig. 4.1.2, it is possible to associate the value of C_A (C_S) with the integral of $|\langle x|A\rangle|^2$ ($|\langle x|S\rangle|^2$) from $-L$ to L , and consequently C_A will be smaller than C_S . And, as mentioned anteriorly the two level approximation is valid for the ASCPT, analogous to Eq. 4.1.2, and so applying it, the hamiltonian assumes the final form:

$$\begin{aligned} \hat{H}_{\text{ASCPT+ECPB}} = & -\frac{1}{2} E_{\text{ASCPT}} (1 - 2n_g) \hat{\sigma}_Z + (E_S |S\rangle\langle S| + E_A |A\rangle\langle A|) \\ & + \frac{1}{2} J (1 - 2n_g - \hat{\sigma}_Z) (C_S |S\rangle\langle S| + C_A |A\rangle\langle A| - N_g) \end{aligned} \quad (4.1.7)$$

The superconducting system is also in contact with three different thermal baths, and they are the essential key enabling the implementation of a Maxwell's demon using this platform. Based on the original concept proposed by Maxwell, the dynamics of the system is investigated in such a way to find a regime of operation in which there will exist a spontaneous heat flux from the colder thermal bath, at the left end of the ASCPT, to the hotter thermal bath, at the right end of the ASCPT. In the proposed implementation, the role of the demon, responsible for mediating this heat flux without performing work, is assumed by the superconducting island of the ASCPT and by the ECPB. So, as expected from a Maxwell's demon, the consequence of the aforementioned heat flux is the decrease of the total entropy of both left and right baths at the end of the ASCPT, resulting in an apparent "violation" of the 2nd law of thermodynamics. However, this "violation" only stands if the variation of entropy of the bath coupled to our ECPB is not taken in account. To create this described heat flux, from the cold to the hot bath, heat will be necessarily released to this third bath, resulting in an increase of its entropy. Therefore, the entropy of the total system, which encompasses the three baths, will increase and the 2nd law will be in the end, satisfied.

4.2 Structure of the energy levels of the superconducting device

At this point is essential to explain how this heat flow, that apparently "violates" the 2nd law can be generated in the described system. The key point is that the Cooper pairs that are in the reservoirs will tunnel through the ASCPT only if assisted by the baths. That is, the last occupied energy levels of the reservoirs are not in resonance with the energy levels of the island of the ASCPT, therefore for Cooper pairs to tunnel from or to the left (or right) reservoir, heat must be absorbed or released to the bath at the left (or right) end of the ASCPT. In Fig. 4.2.1 we represent the general idea underlying the concept for the operation of the demon. Initially the state of the demon is $|0, S\rangle$, that is, the island has no excess charge and the ECPB is in the symmetric state. Then, a Cooper pair tunnels from the left reservoir to the island, absorbing heat Q from the cold bath at the left, which corresponds to the transition $1 \rightarrow 2$, as represented in Fig. 4.2.1. In sequence, the feedback action of the demon occurs, which is characterized by the change of state of the ECPB from symmetric to antisymmetric, corresponding to the transition $2 \rightarrow 3$. This is associated with heat being released to the bath in contact with the ECPB and the change in the configuration of the energy levels of the island. And then occurs the transition $3 \rightarrow 4$, where the Cooper pair tunnels from the island to the right reservoir, releasing the same amount of heat, Q , to the hot bath at the right. For the last, the state of the ECPB changes again, back to symmetric, releasing heat to the bath with which it is in contact, called as the "reset" in Fig. 4.2.1. Note that in this way, the state of the demon at the beginning is the same as in the end of the process. So, heat Q has been transferred from a cold to a hot bath because of the action of the demon and it is important to stress that the demon has not

Table 4.2 – Transitions between states caused by each one of the baths

Bath T $\{\}_T$	Bath T_l $\{\}_T$	Bath T_r $\{\}_T$
$ 1\rangle \leftrightarrow 2\rangle$	$ 1\rangle \leftrightarrow 5\rangle$	$ 1\rangle \leftrightarrow 3\rangle$
$ 3\rangle \leftrightarrow 4\rangle$	$ 2\rangle \leftrightarrow 6\rangle$	$ 2\rangle \leftrightarrow 4\rangle$
$ 5\rangle \leftrightarrow 6\rangle$	$ 3\rangle \leftrightarrow 7\rangle$	$ 5\rangle \leftrightarrow 9\rangle$
$ 7\rangle \leftrightarrow 8\rangle$	$ 4\rangle \leftrightarrow 8\rangle$	$ 6\rangle \leftrightarrow 10\rangle$
$ 9\rangle \leftrightarrow 10\rangle$	–	–

Source: By the author

done work during the process, as its feedback action is associated only with internal changes in its energy levels and the interaction with the baths itself are associated just with heat exchange. And also, it is essential to note that the demon has not effectively exchanged heat with the baths, as the same amount of heat absorbed from the cold bath is released to the hot one. The demon was just responsible for mediating this heat flux through the control of the tunneling processes of Cooper pairs.

In order to further investigate the above described tunneling of Cooper pairs, the complete hamiltonian of the superconducting device must be obtained. This total hamiltonian, $\hat{H}$, includes the already described hamiltonian of the elements that compose the demon, $\hat{H}_{\text{ASCPT+ECPB}}$, and also must account for the energy differences caused by the potential bias, battery, along the ASCPT. That is, if a Cooper pair tunnels from one of the reservoirs to the island in the direction (or against) the potential, there will be an extra energy cost equal to $-eV/2$ ($eV/2$). To correctly account for these energy differences, we add to the description of our state variables giving the number of Cooper pairs in the left and right reservoirs, respectively n_l and n_r . The state of the system is now defined as $|n_l, 0(\text{or } 1), n_r, S(\text{or } A)\rangle$ and the existence of this bias breaks the degeneracy among states where no Cooper pair has tunneled and the ones where a pair has successfully tunneled from the left (right) to the right (left) reservoir. This is, as example, the states $|n_l, 0, n_r, S\rangle$, $|n_l - 1, 0, n_r + 1, S\rangle$ and $|n_l + 1, 0, n_r - 1, S\rangle$ no longer have the same energy. The investigation addressed in this work is for the tunneling of just one Cooper pair, so in this case, considering charge conservation, the states that describe in totality the dynamics are: $|1\rangle \equiv |n_l, 0, n_r, A\rangle$, $|2\rangle \equiv |n_l, 0, n_r, S\rangle$, $|3\rangle \equiv |n_l, 1, n_r - 1, A\rangle$, $|4\rangle \equiv |n_l, 1, n_r - 1, S\rangle$, $|5\rangle \equiv |n_l - 1, 1, n_r, A\rangle$, $|6\rangle \equiv |n_l - 1, 1, n_r, S\rangle$, $|7\rangle \equiv |n_l + 1, 0, n_r - 1, A\rangle$, $|8\rangle \equiv |n_l + 1, 0, n_r - 1, S\rangle$, $|9\rangle \equiv |n_l - 1, 0, n_r + 1, A\rangle$ and $|10\rangle \equiv |n_l - 1, 0, n_r + 1, S\rangle$. As a matter of example, in this representation, from state $|1\rangle$ to $|5\rangle$, a Cooper pair has tunneled from the left reservoir to the island of the ASCPT, absorbing or releasing heat to the left bath. In Tab. 4.2 all the transitions between these above described states, caused by the three baths, are made explicit.

As all the transitions between these ten states are mediated by the baths, the total hamiltonian

Figure 4.2.1 – Schematic representation of the operation of the proposed Maxwell's demon, which is responsible for mediating a heat flux from a colder bath to a hotter bath. When a Cooper pair tunnels from the left reservoir to the island of the ASCPT, heat Q is absorbed from the cold bath T_l ($1 \rightarrow 2$). Then, the demon applies a feedback action, upon the detection of this tunneling, that is characterized by the change of state of the ECPB from symmetric to antisymmetric. During this process ($2 \rightarrow 3$) heat is released to bath T . In the sequence, the Cooper pair tunnels from the island to the right reservoir, and heat Q is released to the hot bath T_r ($3 \rightarrow 4$). For the last, the demon again applies its feedback action characterized now by the change of state of the ECPB, from antisymmetric back to symmetric (reset), releasing heat to the bath T .

Source: By the author

Table 4.3 – Values of the energy gaps for the hamiltonian $\hat{H}$ (note that the hamiltonian $\hat{H}_{\text{ASCPT}+\text{ECPB}}$ is abbreviated as $\hat{H}_{\text{ASC}\dots}$ to fit in the table)

Energy gaps for $\hat{H}$	Values
$\langle 1 \hat{H} 1\rangle - \langle 2 \hat{H} 2\rangle$	$\langle 0,A \hat{H}_{\text{ASC}\dots} 0,A\rangle - \langle 0,S \hat{H}_{\text{ASC}\dots} 0,S\rangle$
$\langle 6 \hat{H} 6\rangle - \langle 2 \hat{H} 2\rangle$	$(\langle 1,S \hat{H}_{\text{ASC}\dots} 0,S\rangle - \frac{1}{2}eV) - \langle 0,S \hat{H}_{\text{ASC}\dots} 0,S\rangle$
$\langle 6 \hat{H} 6\rangle - \langle 5 \hat{H} 5\rangle$	$(\langle 1,S \hat{H}_{\text{ASC}\dots} 1,S\rangle - \frac{1}{2}eV) - (\langle 1,A \hat{H}_{\text{ASC}\dots} 1,A\rangle - \frac{1}{2}eV)$
$\langle 5 \hat{H} 5\rangle - \langle 9 \hat{H} 9\rangle$	$(\langle 1,A \hat{H}_{\text{ASC}\dots} 1,A\rangle - \frac{1}{2}eV) - (\langle 0,A \hat{H}_{\text{ASC}\dots} 0,A\rangle - eV)$
$\langle 9 \hat{H} 9\rangle - \langle 10 \hat{H} 10\rangle$	$(\langle 0,A \hat{H}_{\text{ASC}\dots} 0,A\rangle - eV) - (\langle 0,S \hat{H}_{\text{ASC}\dots} 0,S\rangle - eV)$
$\langle 7 \hat{H} 7\rangle - \langle 8 \hat{H} 8\rangle$	$(\langle 0,A \hat{H}_{\text{ASC}\dots} 0,A\rangle + eV) - (\langle 0,S \hat{H}_{\text{ASC}\dots} 0,S\rangle + eV)$
$\langle 4 \hat{H} 4\rangle - \langle 8 \hat{H} 8\rangle$	$(\langle 1,S \hat{H}_{\text{ASC}\dots} 0,S\rangle + \frac{1}{2}eV) - (\langle 0,S \hat{H}_{\text{ASC}\dots} 0,S\rangle + eV)$
$\langle 4 \hat{H} 4\rangle - \langle 3 \hat{H} 3\rangle$	$(\langle 1,S \hat{H}_{\text{ASC}\dots} 1,S\rangle + \frac{1}{2}eV) - (\langle 1,A \hat{H}_{\text{ASC}\dots} 1,A\rangle + \frac{1}{2}eV)$
$\langle 3 \hat{H} 3\rangle - \langle 1 \hat{H} 1\rangle$	$(\langle 1,A \hat{H}_{\text{ASC}\dots} 1,A\rangle + \frac{1}{2}eV) - \langle 0,A \hat{H}_{\text{ASC}\dots} 0,A\rangle$

Source: By the author

$\hat{H}$, is diagonal in this base. So, with the values for the hamiltonian of the ASCPT and the ECPB, Eq. 4.1.7 and adding the energy differences associated with the bias, $\pm eV/2$, it is obtained that the energy gaps between the states are as given in Tab. 4.3. So taking state $|1\rangle$ as to be the 0 of energy, $\hat{H}$ is given as:

$$\begin{aligned}
 \hat{H} = & 0|1\rangle\langle 1| - Q_2|2\rangle\langle 2| + \varepsilon_2|3\rangle\langle 3| + (\varepsilon_2 + Q_1)|4\rangle\langle 4| \\
 & - (Q_1 + Q_2 - \varepsilon_1)|5\rangle\langle 5| - (Q_2 - \varepsilon_1)|6\rangle\langle 6| + eV|7\rangle\langle 7| \\
 & + (eV - Q_2)|8\rangle\langle 8| - eV|9\rangle\langle 9| - (eV + Q_2)|10\rangle\langle 10|
 \end{aligned} \tag{4.2.1}$$

where we defined:

$$Q_1 = E_S - E_A + J(1 - n_g)(C_S - C_A) \tag{4.2.2}$$

$$Q_2 = E_A - E_S - Jn_g(C_A - C_S) \tag{4.2.3}$$

$$\varepsilon_1 = E_{\text{ASCPT}}(1 - 2n_g) + J(C_S - N_g) - \frac{1}{2}eV \tag{4.2.4}$$

$$\varepsilon_2 = E_{\text{ASCPT}}(1 - 2n_g) + J(C_A - N_g) + \frac{1}{2}eV \tag{4.2.5}$$

As outlined in Fig. 4.2.1 the heat absorbed from the cold bath when a Cooper pair tunnels from the left reservoir to the island (and the ECPB is in the symmetric state), must be the same as the one released in the hot bath, when a pair tunnels from the island to the right reservoir (and the ECPB

is in the antisymmetric state). This is, the energy gaps, between states $|6\rangle$ and $|2\rangle$, that is ε_1 , and between states $|5\rangle$ and $|9\rangle$, that is ε_2 , must be equal and will be denoted as Q . This requirement imposes a direct condition on the value of the externally controlled potential bias, that must be satisfied during the whole operation of the demon:

$$\varepsilon_1 = \varepsilon_2 \equiv Q \Rightarrow eV = J\Delta C \quad (4.2.6)$$

where ΔC is defined as $C_S - C_A$ and thus it is obtained that :

$$Q = E_{\text{ASCPT}}(1 - 2n_g) + J(C_S + C_A - N_g) \quad (4.2.7)$$

So we can now schematically represent the energy levels of $\hat{H}$, as in Fig. 4.2.2. The validity of this representation, that will be precious in the future phenomenological analysis of the dynamics of the device, assumes that the condition $Q_1 > Q_2 > Q > 0$ is satisfied. For this to be true, the values for the gate charges, also externally controlled, must obey some conditions depending on the other parameters of the problem. For n_g :

$$\frac{\Delta E}{J\Delta C} < n_g < \frac{1}{2} + \frac{\Delta E}{J\Delta C} \quad (4.2.8)$$

where ΔE is defined as $E_S - E_A$. And for N_g , depending also on n_g :

$$C_S - \frac{\Delta C}{2} + \frac{E_{\text{ASCPT}}}{J}(1 - 2n_g) + \frac{\Delta E}{J} - n_g\Delta C < N_g < C_S - \frac{\Delta C}{2} + \frac{E_{\text{ASCPT}}}{J}(1 - 2n_g) \quad (4.2.9)$$

Now a first phenomenological approach for the dynamics can be carried. Based on it, it is possible to check if, with the above deduced hamiltonian, a Maxwell's demon can be really implemented using the superconducting device. Also, it enables us to define conditions for the temperatures and transitions rates of the baths in such a way that the dynamics is as the one desired. All possible transitions between states were made explicit in Tab. 4.2 and just single quantum number transitions are considered in the dynamics. This is, transitions in which either the state of the ASCPT has changed, or the state of the ECPB has changed, in other words, simultaneous transitions caused by more than one bath are not considered. As a matter of example, as mentioned, all transitions in Tab. 4.2 are single quantum number transitions, however the transition from $|2\rangle$ to $|3\rangle$ is not.

In this way, suppose the initial state as being $|2\rangle$. According to Tab. 4.2, the transitions allowed are to states $|1\rangle$, $|4\rangle$ or $|6\rangle$. However, if we impose that, see Fig. 4.2.2:

Figure 4.2.2 – Representation of the ten energy levels of $\hat{H}$, that describes the superconducting device considering the energy differences caused by the existence of the voltage bias. The dynamics is started in state $|2\rangle$, where there is no excess or lack of Cooper pairs in the reservoirs, and the ECPB is in state $|S\rangle$ and the ASCPT in state $|0\rangle$. The transitions that occur in the desired process are represented in pink and dotted arrows: $|2\rangle \rightarrow |6\rangle \rightarrow |5\rangle \rightarrow |9\rangle \rightarrow |10\rangle$. The final state is $|10\rangle$ where there is one excess electron in the right reservoir and the ECPB and the ASCPT are in the same states as initially. During this process, heat Q is absorbed from the cold bath, at the left of the ASCPT, and released to the hot bath, at the right of the ASCPT. Also, heat $Q_1 + Q_2$ is released to the bath in contact with the ECPB. It is that $eV = J\Delta C$ and that $Q_1 > Q_2 > Q > 0$.

Source: By the author

$$k_B T \ll Q_2 \quad (4.2.10)$$

$$k_B T_l \sim Q \quad (4.2.11)$$

$$k_B T_r \ll Q + Q_1 + Q_2 \quad (4.2.12)$$

the occupation of the higher energy levels of $\hat{H}$, $|1\rangle$, $|3\rangle$, $|4\rangle$, $|7\rangle$ and $|8\rangle$, is prevented, since it is not desired that they participate on the dynamics. And so, the transition to $|6\rangle$ will be much more probable, which is associated with heat Q being absorbed from the bath at the left of the ASCPT, corresponding to the desired process $1 \rightarrow 2$ as represented in Fig. 4.2.1. Note that the conditions required for the temperatures, Eq. 4.2.10 to Eq. 4.2.12, suggest that $T < T_l$, and as by construction of our problem we impose that $T_l < T_r$, we obtain the given relation for the temperatures of the baths:

$$T < T_l < T_r \quad (4.2.13)$$

From $|6\rangle$, the allowed transitions are back to state $|2\rangle$ or to states $|5\rangle$ and $|10\rangle$. If the relaxation rate associated with the bath in contact with the ECPB for the transition $|6\rangle \rightarrow |5\rangle$, denoted by $\Gamma_{(5 \rightarrow 6)_T}^-$, is much higher in comparison with the relaxation rate associated with the bath coupled to the right end of the ASCPT for the transition $|6\rangle \rightarrow |10\rangle$, denoted by $\Gamma_{(10 \rightarrow 6)_{T_r}}^-$, this is:

$$\Gamma_{(10 \rightarrow 6)_T}^- \ll \Gamma_{(5 \rightarrow 6)_{T_r}}^- \quad (4.2.14)$$

the transition to $|5\rangle$ will occur with a higher probability and will be associated to the release of heat Q_1 to the bath in contact with the ECPB. This transition corresponds to the process $2 \rightarrow 3$, Fig. 4.2.1. From state $|5\rangle$, the allowed transitions are back to $|6\rangle$ or to $|9\rangle$. As already required in Eq. 4.2.10, and as $Q_1 > Q_2$, we automatically have that $k_B T \ll Q_1$ and the transition to state $|9\rangle$ will be more probable. Associated with it, heat Q will be released to the bath at the right side of the ASCPT, corresponding to the process $3 \rightarrow 4$, Fig. 4.2.1. For the last, from state $|9\rangle$ the allowed transitions are back to $|5\rangle$ or to $|10\rangle$, and the transition to the lower energy state $|10\rangle$ is more probable, being associated with the release of heat Q_2 to the bath in contact with the ECPB. From state $|10\rangle$, it could transition back to $|9\rangle$ or to $|6\rangle$, but conditions Eq. 4.2.10 and Eq. 4.2.12 imply that this transitions are not favored by the bath, and the device will tend to stay in $|10\rangle$, thus reaching a steady state. By the fact that in state $|10\rangle$, the ASCPT and the ECPB returned to the same state as in $|2\rangle$, a new cycle of operation will begin, with another Cooper pair tunneling from the left to the right reservoir and heat Q again being absorbed from a cold bath and then released to a hot bath.

So, in this initial analysis we can conclude that if certain conditions are fulfilled, the main process occurring during the dynamics is:

$$|2\rangle \rightarrow |6\rangle \rightarrow |5\rangle \rightarrow |9\rangle \rightarrow |10\rangle \quad (4.2.15)$$

and as desired, the tunneling of Cooper pairs is such that heat Q will be transported from the cold to the hot bath, and heat $Q_1 + Q_2$ is released to the bath in contact with the ECPB. It is important to emphasize that, as expected, energy is conserved during the process in the total system, which englobes the superconducting device, the baths and also the battery. This is true because the total heat delivered to the bath of temperature T is equal to eV , Eqs. 4.2.2, 4.2.3 and 4.2.6, which is exactly equal to the difference in energy between the Cooper pairs in the left and right reservoirs. Note however that, although the battery is as essential element to the functioning of the device as a Maxwell's demon, it does not realize work, as the transitions between the states are always assisted by the baths.

Thus, as the state of the demon is the same at the beginning and at the end of the described process, the total variation of entropy is given in terms only of the variation of entropy of the baths, simply defined as $\Delta S_B = \Delta Q_B/T$, this is the ratio between the heat gained by the bath and its temperature. Therefore we have that the variation of entropy for the left, cold, bath and for the right, hot, bath, defined as $\Delta S_{\text{Baths } T_l \& T_r}$ is negative and equal to:

$$\begin{aligned} \Delta S_{\text{Baths } T_l \& T_r} &= Q \left(\frac{1}{T_r} - \frac{1}{T_l} \right) \\ &= \left[E_{\text{ASCPT}}(1 - 2n_g) + \frac{1}{2}J(C_S + C_A - 2N_g) \right] \left(\frac{1}{T_r} - \frac{1}{T_l} \right) < 0 \end{aligned} \quad (4.2.16)$$

The variation of entropy of the bath in contact with the ECPB, defined as $\Delta S_{\text{Bath } T}$, is given by:

$$\Delta S_{\text{Bath } T} = \frac{1}{T} (Q_1 + Q_2) \quad (4.2.17)$$

$$= \frac{1}{T} J \Delta C \quad (4.2.18)$$

And the total variation of entropy, encompassing all three baths, defined as ΔS_{Baths} , is given by:

$$\begin{aligned}
\Delta S_{\text{Baths}} &= \Delta S_{\text{Bath } T} + \Delta S_{\text{Baths } T_l \& T_r} \\
&= (Q_1 + Q_2) \frac{1}{T} - Q \left(\frac{1}{T_l} - \frac{1}{T_r} \right) > 0
\end{aligned} \tag{4.2.19}$$

It is important to note that, as expected by the validity of the 2nd law, ΔS_{Baths} assumes a positive value. It is easy to see this because, as mentioned anteriorly and represented in Fig. 4.2.2, $Q_1 + Q_2 > Q$. And also, the condition obtained for the temperatures, 4.2.13, consequently impose that $\frac{1}{T} > \frac{1}{T_l} - \frac{1}{T_r}$, so it is guaranteed that $\Delta S_{\text{Bath } T} > -\Delta S_{\text{Baths } T_l \& T_r}$.

At this point, it could be argued that the variation of entropy here calculated is not complete, as only the heat flow is being considered and not the matter flow. However, the crucial point is that the matter flow is constituted of Cooper pairs and when pairs tunnel from the left to the right reservoir there is no entropy change associated with this matter flow. This is true because in each reservoir, Cooper pairs, which are bosons, are all condensed in the fundamental superconducting state, characterizing a pure state which has entropy equal to zero. When a pair tunnels out of the left reservoir, the pairs left in the reservoir are still all condensed to the fundamental superconducting state, and there will be no entropy change. When a pair tunnels in the right reservoir it will also be in a condensed state, and there will be also no entropy change to the reservoir. Note that the energy and temperature scales are small compared to the superconducting gap such that Cooper pairs are not broken, and the tunneling dynamics may be described only in terms of Cooper pairs.

4.3 Dynamics of the superconducting device

However, to verify if the above described process, Eq. 4.2.15, will really occur, it is necessary to determine the dynamics of the density matrix describing the device, $\hat{\rho}(t)$. The quantum master equation of the system was constructed in a phenomenological way, and the interaction with the baths is described in the Lindblad form (51):

$$\begin{aligned}
\frac{d\hat{\rho}(t)}{dt} = & -\frac{i}{\hbar} [\hat{H}, \hat{\rho}(t)] + \\
& \sum_{\{T\}} \left\{ \Gamma_{(i \rightarrow j)_T}^+ \mathcal{D}[|j\rangle\langle i|] \hat{\rho}(t) + \Gamma_{(i \rightarrow j)_T}^- \mathcal{D}[|i\rangle\langle j|] \hat{\rho}(t) \right\} + \\
& \sum_{\{T_l\}} \left\{ \Gamma_{(i \rightarrow j)_{T_l}}^+ \mathcal{D}[|j\rangle\langle i|] \hat{\rho}(t) + \Gamma_{(i \rightarrow j)_{T_l}}^- \mathcal{D}[|i\rangle\langle j|] \hat{\rho}(t) \right\} + \\
& \sum_{\{T_r\}} \left\{ \Gamma_{(i \rightarrow j)_{T_r}}^+ \mathcal{D}[|j\rangle\langle i|] \hat{\rho}(t) + \Gamma_{(i \rightarrow j)_{T_r}}^- \mathcal{D}[|i\rangle\langle j|] \hat{\rho}(t) \right\} \quad (4.3.1)
\end{aligned}$$

where we define the collapse superoperator as $\mathcal{D}[\hat{\mathcal{A}}] \hat{\rho}(t) = \hat{\mathcal{A}} \hat{\rho}(t) \hat{\mathcal{A}}^\dagger - \frac{1}{2} \{ \hat{\mathcal{A}}^\dagger \hat{\mathcal{A}}, \hat{\rho}(t) \}$. The transition from state i to j , with respective eigenenergies E_i and E_j , $E_i < E_j$, is represented by the operator $|j\rangle\langle i|$, and the sets of all possible transitions caused by each bath are described in Tab. 4.2 and represented as $\{T\}$, $\{T_l\}$ and $\{T_r\}$. The relaxation and excitation rates, for the transition $i \rightarrow j$, are respectively defined as $\Gamma_{(i \rightarrow j)_b}^-$ and $\Gamma_{(i \rightarrow j)_b}^+$, where the subindex b assumes a different notation for each bath: T , for the transitions caused by the bath in contact with the ECPB, T_l , for the transitions caused by the bath at the left end of the ASCPT and T_r , for the transitions caused by the bath at the right end of the ASCPT. Also, the rates satisfy the relation $\Gamma_{(i \rightarrow j)_b}^+ = \Gamma_{(i \rightarrow j)_b}^- e^{-\beta_b(E_j - E_i)}$, where for b equal to T , T_l and T_r , respectively, $\beta_T = 1/k_B T$, $\beta_{T_l} = 1/k_B T_l$ and $\beta_{T_r} = 1/k_B T_r$.

The approach taken to analyze the dynamics is to begin with a initial density matrix in the pure state $\hat{\rho}(0) = |2\rangle\langle 2|$ and analyze the evolution of the probabilities of occupation of each one of the 10 states, $P_i(t) = \langle i | \hat{\rho}(t) | i \rangle$ during the dynamics. Note that this initial state corresponds to $\hat{\rho}(0) = \hat{\rho}_{\text{ASCPT}}(0) \otimes \hat{\rho}_{\text{ECPB}}(0)$, with $\hat{\rho}_{\text{ASCPT}}(0) = |n_l, 0, n_r\rangle\langle n_l, 0, n_r|$ and $\hat{\rho}_{\text{ECPB}}(0) = |S\rangle\langle S|$. In this way, it is possible to verify if the states occupied are the ones desired, if the higher energy states do not participate in the dynamics and also if a steady state is reached. To numerically solve Eq. 4.3.1, all the parameters of the problem assume experimentally feasible values directly based on the ones contained in. (1) In this way, the charging energy of the ASCPT is equal to $E_{\text{ASCPT}}/k_B = 1.7$ K and the eigenenergies of the antisymmetric and symmetric states of the ECPB are respectively given by $E_A/k_B = 800$ mK and $E_S/k_B = 780$ mK. The coupling strength between them assumes the value $J/k_B = 500$ mK and the terms controlling the difference between the coupling of the antisymmetric and symmetric states with the ASCPT are equal to $C_A = 0.1$ and $C_S = 0.9$. Consequently, as explicit in condition given by Eq. 4.2.6, $eV/k_B = 400$ mK. In order to satisfy conditions contained in Eq. 4.2.8 and Eq. 4.2.9, the values of the gates charges are chosen as equal to $n_g = 0.44$ and $N_g = 0.85$.

So based on the values explicit in Tab. 4.4, the heat exchanged with the baths, as defined in Eqs. 4.2.2, 4.2.3 and 4.2.7, are equal to $Q/k_B = 29$ mK, $Q_1/k_B = 204$ mK and $Q_2/k_B = 196$ mK. Now,

Table 4.4 – Values of all physical parameters associated with the superconducting device analyzed and that were used to perform the numerical simulations

Parameters	Values
E_{ASCPT}/k_B	1.7 K
E_A/k_B	800 mK
E_S/k_B	780 mK
J/k_B	500 mK
C_A	0.1
C_S	0.9
eV/k_B	400 mK
n_g	0.44
N_g	0.85

Source: By the author

with these values, the temperatures of the three baths are chosen in order to satisfy the conditions described anteriorly that guarantee the desired dynamics, Eqs. 4.2.10 to 4.2.13. So, they assume the given values $T = 20$ mK, $T_l = 25$ mK and $T_r = 30$ mK. For the last, the relaxation rates for all the transitions caused by the baths at the left and right end of the ASCPT are taken as equal, being defined respectively as $\Gamma_{T_l}^-$ and $\Gamma_{T_r}^-$, and are equal to 10^8 Hz. Also, the relaxation rates for the transitions caused by the bath in contact with the ECPB are also taken as equal, being defined as Γ_T^- , and as to satisfy the condition explicit in Eq. 4.2.14 assume the value of 10^9 Hz.

Table 4.5 – Values of the parameters associated with the baths in contact with the superconducting device

Parameters	Values
Q_1/k_B	204 mK
Q_2/k_B	196 mK
Q/k_B	29 mK
T	20 mK
T_l	25 mK
T_r	30 mK
$\Gamma_{T_l}^-$	10^8 Hz
$\Gamma_{T_r}^-$	10^8 Hz
Γ_T^-	10^9 Hz

Source: By the author

Therefore, using the values explicit in Tabs. 4.4 and 4.5, the numerically determined time evolution of the probabilities of occupation of the states is represented in Fig. 4.3.1. It is obtained that the probability of occupation for the state $|2\rangle$, defined as P_2 , evolves from 1 to 0. And the occupation of state $|10\rangle$, defined as P_{10} , evolves from 0 to 1, showing that this is the stationary state of the device.

Figure 4.3.1 – Evolution of the probabilities of occupation, P_i , of the states $|i\rangle$, during the dynamics

Source: By the author

Also, it is possible to see in Fig. 4.3.1 and in more details in Fig. 4.3.2, that states $|6\rangle$, $|5\rangle$ and $|9\rangle$ are occupied during the dynamics in this given order. For the last, in Fig. 4.3.3, it is noticed that the probabilities of occupation of all the higher energy states not desired to participate in the dynamics, $|1\rangle$, $|3\rangle$, $|4\rangle$, $|7\rangle$ and $|8\rangle$, are indeed very low, of order of 10^{-5} or lower. It is of supreme importance

Figure 4.3.2 – Evolution of the probabilities of occupation of states $|5\rangle$, $|6\rangle$ and $|9\rangle$ during the dynamics

Source: By the author

to note that all the dynamics occurs in a time scale of 200 ns, for which the quantum features of the device, including the entanglement between the CPB's, can be experimentally maintained.

This is, the dynamics begins in the pure state $|2\rangle\langle 2|$ and ends also in the pure state $|10\rangle\langle 10|$, also occupying $|6\rangle$, $|5\rangle$ and $|9\rangle$ during the evolution, being that the other states effectively do not participate in the dynamics. So, conclusions, based on these results, about the heat exchanged with the baths during the dynamics, depend on the analysis of all possible processes that connect states $|2\rangle$ and $|10\rangle$, passing through $|6\rangle$, $|5\rangle$ or $|9\rangle$. Based on Tab. 4.2, there are 2 of them, being that the first one is described in Eq. 4.2.15 and is exactly the desired process characteristic of the behavior of the demon and already discussed in detail. However, there also exists this second process, given as:

$$|2\rangle \rightarrow |6\rangle \rightarrow |10\rangle \quad (4.3.2)$$

where there is no change in the state of the ECPB. As can be seen in Fig. 4.2.2, in the transition from $|2\rangle$ to $|6\rangle$ heat Q is absorbed from the bath at the left end of the ASCPT and in the transition from $|6\rangle$ to $|10\rangle$, heat $Q_1 + Q_2 + Q$ is released to the hot bath at the right end of the ASCPT. Note that, if this process actually occurs during the dynamics, there is no feedback action of the demon, which is precisely associated with the change of state of the ECPB, and although a given amount of heat is absorbed from a cold bath, and a different amount of heat is released to a hot bath, the entropy variation caused by this process is not negative. This can be easily seen by the fact that this entropy variation is defined as:

$$\frac{(Q_1 + Q_2 + Q)}{T_r} - \frac{Q}{T_l} \quad (4.3.3)$$

and for this quantity to be negative, $Q_1 + Q_2 + Q \ll k_B T_r$ as Eq. 4.2.11 imposes that $k_B T_l \sim Q$. However, the other existent condition, Eq. 4.2.12, imposes exactly the opposite, so this variation of

Figure 4.3.3 – Evolution of the probabilities of occupation of states $|1\rangle$, $|3\rangle$, $|4\rangle$, $|7\rangle$ and $|8\rangle$ during the dynamics
Source: By the author

entropy must be actually positiveⁱ.

Despite the existence in the dynamics of this undesired process, Eq. 4.3.2, the condition in Eq. 4.2.14, precisely imposes that the transition from state $|6\rangle$ directly to $|10\rangle$, is much less likely to happen than the transition to state $|5\rangle$. Therefore, the main process occurring is actually the desired one, characteristic of the demon. To verify this statement, the dynamics was simulated as in Eq. 4.3.1, however excluding the undesired direct transition $|6\rangle \leftrightarrow |10\rangle$. So, representing the density matrix in this case as $\hat{\rho}'(t)$, where it is also assumed that $\hat{\rho}'(0) = |2\rangle\langle 2|$, the probabilities of occupation for the dynamics without the undesired process, defined as $P'_i = \langle i | \hat{\rho}'(t) | i \rangle$, are compared with the probabilities P_i , obtained previously.

By the analysis of Fig. 4.3.4, it is possible to see that the deviation of P'_i in comparison with the values of P_i is of order of 10% or less for all the ten states. So the undesired process indeed occurs, however its influence in the dynamics is small. Therefore, it is fair to affirm that the obtained results show that the dynamics is such that the desired process, represented in Fig. 4.2.1 and outlined in Eq. 4.2.15, occurs in a higher proportion than the undesired one and consequently the dynamics of the device can be characterized in fact as a Maxwell's demon. And using expression Eq. 4.2.16, the negative variation of entropy of the baths can be calculated, considering the values in Tab. 4.5,

ⁱ This could be also expected by the 2nd law, as this computed variation of entropy is the variation of entropy of all baths during the dynamics, because there is no heat exchanged with the bath in contact with the ECPB, and so, it must be positive.

Figure 4.3.4 – Comparison between the probabilities of occupation when the undesired process, $|6\rangle \leftrightarrow |10\rangle$, is removed from the dynamics

Source: By the author

being equal to:

$$\Delta S_{\text{Baths } T_l \& T_r} \simeq -0.19 k_B \quad (4.3.4)$$

Also, considering Eq. 4.2.17, the expected positive variation of entropy of the bath in contact with the demon is equal to:

$$\Delta S_{\text{Bath } T} = 20 k_B \quad (4.3.5)$$

This is, as expected the demon is responsible for decreasing the entropy of the baths at the end of the ASCPT without doing any work. However, for the action of the demon to be possible, it must release heat to a bath to which it is in contact, consequently increasing its entropy. And, as expected by the 2nd law, the total variation of entropy is positive, in this case equal to:

$$\Delta S_{\text{Baths}} = \Delta S_{\text{Bath } T} + \Delta S_{\text{Baths } T_l \& T_r} \simeq 19.81 k_B \quad (4.3.6)$$

It is important to mention that the initial state was taken as $|2\rangle\langle 2|$ because this is the most symmetrical option that could be made. In the sense that, in the state $|2\rangle$ no Cooper pair has yet tunneled through the ASCPT, and so there is no excess or lack of pairs in the reservoirs. Also, in state $|2\rangle$ the ECPB is already set to its desired initial state, $|S\rangle$, ready to detect the tunneling of a Cooper pair from the left reservoir to the island of the ASCPT. However, the dynamics has been also numerically obtained taking as initial state all the others possible pure states, that is, $|1\rangle\langle 1|$,

$|3\rangle\langle 3|$, $|4\rangle\langle 4|$, $|5\rangle\langle 5|$, $|6\rangle\langle 6|$, $|7\rangle\langle 7|$, $|8\rangle\langle 8|$, $|9\rangle\langle 9|$ and $|10\rangle\langle 10|$. For all them it was verified that the final stationary state for the dynamics is state $|10\rangle$. So, if the initial state is $|1\rangle$, it was verified that the main process occurring during the dynamics is:

$$|1\rangle \rightarrow |2\rangle \rightarrow |6\rangle \rightarrow |5\rangle \rightarrow |9\rangle \rightarrow |10\rangle \quad (4.3.7)$$

and the desired behavior of a demon is obtained, but with extra heat Q_2 being released to the bath in contact with the ECPB in the transition from $|1\rangle$ to $|2\rangle$. For the other possible initial states, the heat exchanges with the baths do not have the desired characteristics of a demon. For example, if the initial state is taken as $|5\rangle$ the main process occurring during the dynamics is:

$$|5\rangle \rightarrow |9\rangle \rightarrow |10\rangle \quad (4.3.8)$$

such that only heat Q will be released to the hot bath and heat Q_2 is released to the bath in contact with the ECPB. However, the fact that the final state is always equal to $|10\rangle$, in which the states of the ASCPT and the ECPB are equal to as in $|2\rangle$, means that then in the next cycle the dynamics will occur as wished. With the only difference that the initial state for this next cycle will be the one in which a Cooper pair has already tunneled from the left reservoir to the right one. Then during this next cycle, another Cooper pair will tunnel from the left to the right reservoir and a process analogous to Eq. 4.2.15 will occur. The only difference is that now all states will be shifted with one less electron at the left reservoir (n_l goes to $n_l - 1$ in Fig. 4.2.2) and with one extra electron at the right reservoir (n_r goes to $n_r + 1$ in Fig. 4.2.2). In this way it is possible to guarantee that the tunneling of the Cooper pair in this next cycle will then entail that heat will be transferred from the cold to the hot reservoir, and the desired behavior of a demon will be obtained. As one cycle takes in order 200 ns to occur, the time for the operation of the device during more than one cycle is compatible with the time scales where coherence and entangled can be maintained in superconducting devices.

So in overall, it was shown and discussed that the described superconducting device is indeed an implementation of an autonomous quantum Maxwell's demon. It is a demon because, as already discussed, it mediates the heat flux from a cold to a hot bath without doing work, apparently "violating" the 2nd law of thermodynamics. It is autonomous because there is no external feedback action necessary to implement the demon, the spontaneous dynamics is such that the typical behavior of a demon is obtained without need of any external element. For the last, it is quantum for the fact that it is implemented in a platform of superconducting qubits, with its dynamics described by quantum mechanics, and possess a genuinely quantum feature, the entanglement between the CPB's. The original results of this research are to be published soon in an article already in preparation.

Chapter 5

Conclusions

In this dissertation we have explored a short history of Maxwell's thought experiment, from the original "birth" of the demon until its ultimate "exorcism". The contribution given by a wide range of different scientists on the evolution of the concept of Maxwell's demon was explained. From Lord Kelvin, who named the "intelligent being" imagined by Maxwell back in 1867 as a demon, and Szilard, who conceived a simpler version of the same problem, Szilard's engine. Mentioning also the work of Smoluchowski, Brillouin, von Neumann and Penrose, who further developed the concept underlying the demon and even attempted to solve the paradox created by this "intelligent being". To the revolutionary contribution of Landauer, with its Landauer's principle, and Bennett, who applied this principle to finally "exorcise" the demon. The classical and quantum proofs of Landauer's principle are presented in details. Also, the works of Zurek and Lloyd on the quantum version of the demon are addressed. Although the discovery that this "intelligent being" does not represent a real threat to the 2nd law, the demon is far from having lost its charm. Decades of investigation on the topic were able to shed light on the special link between information and thermodynamics. In this way, the demon is now understood as the one responsible for collecting information and trading it for thermodynamic advantage. As an example, this advantage could be the creation of a temperature or pressure difference, the creation of a flux of heat from a cold to a hot reservoir or the direct extraction of useful work.

Furthermore it was to be expected that the evolution on the control of nano-mesoscopic systems would spark the interest on implementing Maxwell's demon using experimental platforms. So, we have briefly analyzed the main experiments, where demons are implemented using macromolecules, lasers, particles in a colloid mixture and even a photonic device. Those experiments can differ largely between themselves, as with the demon being autonomous or non-autonomous and with different ways to obtain thermodynamic advantage. However, they all reveal what was foreseen by Bennett in 1982, that the demon process of collecting information and then discarding it will be necessarily associated with an increase in entropy, and the 2nd law remains valid.

In our analysis, special attention was attributed to the work of Pekola's group. (1, 42) They used electronic solid-state systems to create a Szilard's engine and also a demon able to cool part of the device through the use of information. This last implementation served as base and inspiration for the work developed in this master's research, and so it was reviewed with the deepening deserved.

Recently, Maxwell's "intelligent being" has also entered the quantum realm, with diverse experiments implementing quantum versions of the demon. One of the experimental platforms that reached enormous success are superconducting circuits, with diverse experiments being conducted in the last years. And is exactly in this context that our research fits, since this work presents as an original result the implementation of an autonomous quantum Maxwell's demon using superconducting devices. As in Maxwell's original thought experiment, our demon creates a heat flux from a cold to a hot bath without the realization of any work. This action is only possible because the demon is in contact with a third thermal bath. So it is continuously performing its feedback action and releasing heat to this third bath, analogous to the process of continuously erasing its memory.

In our platform, the role of the demon is played by an ECPB, Extended Cooper-Pair Box, and the island of an ASCPT, Asymmetrical Single-Cooper-pair transistor. The ECPB is a device composed of two interacting CPB's, that are in an entangled state being described by their anti-symmetric and symmetric states: $|A\rangle$ and $|S\rangle$. Cooper pairs can tunnel to the island of the ASCPT coming from left and right reservoirs of pairs, and the island assumes states with occupation equal to zero or one: $|0\rangle$ or $|1\rangle$. The tunneling of the Cooper pairs through the ASCPT is only possible because of thermal excitations of the left, cold, and the right, hot, thermal baths associated respectively with the left and right reservoirs. Also, the ECPB and the ASCPT interact capacitively, such that when a Cooper pair tunnels to the island, which is analogous to the step of the collection of information by the demon, the ECPB then changes its state. This step is analogous to the feedback action of the demon, and its result is to control the tunnel of the Cooper pairs in a preferred direction, without doing any work. This direction is from the left to the right reservoirs, and it is precisely these tunneling events that creates the desired heat flux from the cold to the hot thermal bath. As expected, the Clausius statement of the 2nd law is not violated, as the entropy of the third bath is increased during the process.

It is important to mention that this work differs from the already existent literature due to the use of an element in an entangled state and by the specific choice of how to obtain thermodynamic advantage, that is, extracting heat from a cold to a hot bath. The results of this master's research are to be published soon. And although this work was done in the realm of theory, the use of experimental feasible values during the simulation of its dynamics shows that it could be in reality experimentally implemented. The duration time of the dynamics, around 200 ns, is such that entanglement and coherence can be achieved in superconducting devices. The temperatures assumed to the baths, not below 20 mK, can be generated and maintained in experimental implementations. The devices

used, essentially interacting Cooper-Pair Boxes, have been investigated and implemented since the late 90's, and much knowledge on the control of them is known.

Thus, as future perspectives it is expected that in the near future the superconducting demon here presented will be experimentally implemented. Also, it would be interesting to numerically simulate the dynamics of the superconducting device for states beyond the ones considered in this work. That is, to consider that the ECPB is initially in a mixed state, $\text{tr}(\hat{\rho}_{\text{ECPB}}^2) \leq 1$, where $\hat{\rho}_{\text{ECPB}}$ stands for the density matrix of the ECPB. Note that in Chapter 4, the ECPB is initially always in a pure state, $\hat{\rho}_{\text{ECPB}} = |A\rangle\langle A|$ or $\hat{\rho}_{\text{ECPB}} = |S\rangle\langle S|$. We precede that in this case the time of duration of the dynamics may be different, probably larger. Giving this, an analysis on the power with which the demon extracts heat from the cold bath and delivers to the hot bath can be constructed. Last, in the case of mixed initial states, it may be also possible to observe that the main processes occurring may be different from the ones for an initial pure state. So, the heat exchanges between the baths may be different and also, in this case, processes beyond the single quantum number ones may be analyzed and included in the dynamics. Further considerations on the establishment of a heat current in the opposite direction of the matter current, would be too an interesting topic to approach.

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