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ENTROPY PRODUCTION IN QUANTUM SYSTEMS

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Resumen

En comparación con otras disciplinas, la termodinámica surgió hace bastante poco. Fue en el siglo XIX, con los trabajos de Carnot sobre máquinas térmicas cuando todo empezó, aunque se tardó décadas en llegar a formalizar las primeras ideas. En este cometido trabajaron autores como Clausius, Lord Kelvin, Planck, Boltzmann, Gibbs... Y dos de los principales resultados de estos investigadores fueron los enunciados de la Segunda ley de la Termodinámica y la introducción del concepto de la entropía.

En concreto, la entropía supuso un gran avance en cuanto al formalismo. Y de la misma forma para la producción de entropía, que es una cantidad resultante de la anterior y con la que se puede enunciar el segundo principio de un modo muy útil y elegante. La importancia de esta cantidad se encuentra en que puede servir para caracterizar la irreversibilidad de un proceso, lo cual resulta de capital importancia en muchos casos. Sin embargo, la definición de entropía no es evidente, aparece por primera vez cuando Clausius enuncia su famoso teorema y en un contexto puramente termodinámico. Tan solo unas décadas más tarde, a finales del mismo siglo XIX, Boltzmann introduce su definición de entropía, aunque esto lo hace desde la perspectiva de la física estadística. En esos momentos apenas se podía vislumbrar la cantidad de trabajo que quedaba por hacer en estos campos y que continúa aún hoy.

Durante el siglo XX los avances continuaron, pero esta vez desde otras disciplinas. Con el surgimiento de la física cuántica y la teoría de la información también aparecieron nuevas definiciones de la entropía. Los autores correspondientes fueron, respectivamente, von Neumann y Shannon. Teniendo en mente todos esos contextos en los que se manifiesta la entropía, cabe preguntarse por la relación entre ellos. Hay casos concretos en los que las propiedades termodinámicas (macroscópicas) de un sistema emergen de un estudio estadístico (microscópico). Se aportarán ejemplos de esto cuando sea oportuno y necesario para el asentamiento de los conceptos. No solo por su papel en el estudio de propiedades macroscópicas conviene interesarse por la producción de entropía, también en la física cuántica es útil para el estudio de máquinas térmicas.

La termodinámica y la física estadística surgieron en décadas cercanas, de manera que su relación ha sido siempre más o menos bien conocida. Sin embargo, aparece un reto al intentar llevar la cuántica al terreno de la termodinámica clásica. Para atacar un problema como ese es necesario tener una cierta conexión teórica entre todas las disciplinas. Es por esto que en se presenta en el segundo capítulo de este trabajo una base de teoría de la información, ya que no es una disciplina que aparece en el plan de estudios y solo unos conceptos concretos son importantes aquí. Con los conocimientos adquiridos en ese capítulo es posible dar una interpretación general de la entropía, más allá de la típica

interpretación de desorden $\equiv$ mucha entropía. De hecho, la interpretación más general y que se emplea a lo largo de todo el trabajo es aquella por la cual la entropía es una medida de la "incertidumbre". Como en el caso de la conexión entre la termodinámica y la estadística, se presenta un ejemplo que conecta la termodinámica y la física estadística con la teoría de la información. En concreto, se plantea el problema del Demonio de Maxwell y se da la idea fundamental de su resolución, también se trata de aportar una visión particular a ese problema.

Con las herramientas desarrolladas ya es posible intentar abordar el estudio de sistemas cuánticos con mayor garantía de llegar a entender realmente lo que se está estudiando. No obstante, aunque la forma de las relaciones es muy similar, no se puede dar un desarrollo muy exhaustivo de la conexión entre la entropía en sistemas cuánticos y la entropía en termodinámica o estadística. Esto se debe a que aún a día de hoy se discute la validez de la entropía de von Neumann y se proponen muchas alternativas más o menos fructíferas.

Con todo lo anterior, se tendrá lo necesario para llegar a una de las partes fundamentales del trabajo, que es la obtención de una relación para la producción de entropía en sistemas cuánticos. Como era de esperar, los autores originales establecieron algunas condiciones para llegar a la relación, pero el resultado es bastante general y de utilidad, además, las herramientas matemáticas necesarias resultan muy asequibles. Y las bases teóricas desarrolladas al principio cobran sentido al tratar de interpretar físicamente esta relación.

El objetivo, teniendo todo lo anterior, es estudiar sistemas físicos reales. Se empieza con un modelo relativamente sencillo, el modelo de Jaynes–Cummings. Se ha elegido este con el objetivo de ilustrar los conceptos sobre la entropía que hasta ese momento se han desarrollado de forma teórica. Al tratarse de un modelo simple de interacción y debido a sus características, no es el más adecuado para estudiar la relación obtenida para la producción de entropía, por lo que se trató un caso más.

Para ilustrar las cantidades que representan la producción de entropía se eligió un modelo que en la literatura ya se utilizó para esto, de manera que se puede comprobar la fiabilidad de los resultados obtenidos. Pero no solo se reprodujeron los resultados, se trató de ir más allá estudiando particularidades la evolución temporal del sistema. La validez y utilidad de la relación que se escogió para la producción de entropía queda comprobada, no solo por comparación con resultados de los autores originales, también desde un punto de vista físico y basado en las interpretaciones que se justificaron en las partes del trabajo anteriores a esta.

Finalmente, se da una introducción a los teoremas de fluctuación. Estos son una extensión de la segunda ley de la termodinámica y un campo de estudio muy reciente (desarrollado sobre todo durante las últimas décadas). La complejidad matemática aumenta, pero también el abanico de situaciones que se pueden estudiar. En este trabajo solo se da una introducción al tema, lo suficiente para aplicar el formalismo a resultados teóricos vistos en las partes anteriores. Además, se llega a un teorema de fluctuación a partir de otros teoremas que se pueden encontrar en la bibliografía. La importancia de los teoremas de fluctuación queda patente para entender su importante papel en la investigación actual.

Contents

CHAPTER 1

INTRODUCTION

Resumen

Antes de hablar de la producción de entropía en sistemas cuánticos es conveniente tener claros los conceptos en contextos más básicos. En lo siguiente se presentan varias ideas, en concreto, se presenta la entropía en las principales disciplinas en las que se trata: termodinámica, estadística, cuántica y teoría de la información. Para esta presentación se ha hecho un repaso histórico, dejando fijadas varias definiciones que son imprescindibles para los desarrollos posteriores. Además, se expone la importancia del estudio de la producción de entropía con algunos ejemplos, dando algunas claves para entender por qué hay tanto interés este concepto.

1.1 HISTORICAL REMARKS

If someone wanted to look for a starting point for studies in the field of thermodynamics and, more specifically, for that magnitude that appears in the title of this work, entropy, without a doubt there would be talk of the works on steam engines of Nicolas Léonard Sadi Carnot, published in 1824. Briefly and assuming that the reader has basic knowledge that is acquired in a degree in Physics, a review will begin by pointing out the influence of this author on the works in thermodynamics and entropy that were developed in following decades [LC74]. And basic and subsequent results will continue to be seen, with the aim of emphasizing what is necessary to develop the following chapters.

Although Carnot did not define the concept of entropy, he laid the foundations for the further development of this concept and, above all, of the second principle of thermodynamics. The importance of his works was noted by Émile Clapeyron, who worked to make the reasoning and theory developed by Carnot more understandable. On this basis, many others began to build the rest of classical thermodynamics. For this work, the contribution of Rudolf Clausius, who was the first to explicitly introduce the concept of entropy (1854), is of great interest:

$$Clausius\ entropy\ :=\ \Delta S_{Cl} = \oint \frac{\delta Q}{T}\ . \tag{1.1}$$

Where δQ is an infinitesimal amount of heat absorbed by a system and extracted from a reservoir at temperature T, being the total process cyclical. That author introduced this concept as a tool to state his well-known theorem, which can be expressed as: $\Delta S_{Cl} \leq 0$.

It is important to note that in the above, only the *Clausius entropy* has been defined, the total entropy of a certain system has not been discussed.

In any basic course of thermodynamics it is shown, by means of the previous theorem, that the entropy variation of a closed system (a system that does not exchange matter with its surroundings) between two states B_1, B_2 and in a reversible process , i.e., a process in which both the system considered and its surroundings can return to their initial state, fulfills:

$$S_2 - S_1 = \int_{B_1}^{B_2} \frac{\delta Q}{T} \ . \tag{1.2}$$

It is also easy to verify that in an irreversible process this equality is not fulfilled, but that it is obtained:

$$S_2 - S_1 > \int_{B_1}^{B_2} \frac{\delta Q}{T} \ . \tag{1.3}$$

Which can be rewritten by defining a quantity that will be added to the right side, this is the entropy production term:

$$S_2 - S_1 = \int_{B_1}^{B_2} \frac{\delta Q}{T} + \Sigma \qquad \Sigma := \text{entropy production.} \tag{1.4}$$

So far, everything needed to enunciate the second principle of thermodynamics in the most convenient way for later developments has been presented. And of all the statements that can be made about this principle, probably the simplest is: the entropy of the universe tends to a maximum. Mathematically: $\Delta S_{univ} \geq 0$.

The term "universe" is used to refer to the system together with its surroundings, so any isolated system is being considered. Therefore, the heat exchange is zero. Thus, the previous relationship can be expressed only with the entropy production:

$$\boxed{\Sigma \geq 0} \tag{1.5}$$

This is what the second principle of thermodynamics is reduced to. It will be of vital importance to take this inequality into account, since it will be one of the main arguments when obtaining a physically acceptable equation for the entropy production in a quantum system.

Surely with this brief review it is not possible to glimpse the physical meaning of the entropy production. Nor would it be surprising if with a more extensive and precise review it is not completely clear, the definition of this quantity and that of entropy are still the object of study and discussion in some cases nowadays. For now, it will be enough to understand entropy production as a way of characterizing the irreversibility of a process. Indeed, according to what has been seen above, in a reversible process: $\Sigma = 0$ is satisfied. And in an irreversible one $\Sigma > 0$. It can even be used to find out how far a process moves away from being reversible, specifically, this idea will be illustrated in a little more detail later (in section, Section 1.3) using the case of a system that performs work between two reservoirs.

The time parameter has not yet been explicitly mentioned in the previous reasoning, but it appears clearly in the concept of reversibility: when talking about the initial state

of a system (in the equation (1.2) it was denoted by B_1) its state is being considered in an instant of past time. Intuitively, a relationship between time, entropy and irreversibility already appears, in short: when a system undergoes an irreversible process, that is, it has led to the creation of entropy, the system cannot be returned to the state it had in a previous instant of time. It is well known that time passes in a single "direction" (nothing and nobody can go to the past). So, really, all processes in nature are irreversible.

It should be noted that entropy production characterizes a process experienced by a system, it does not provide information about the state of that system. But entropy is a state function, that is, it is a magnitude that characterizes the equilibrium state of the system under consideration. Although the concept of "equilibrium" is intuitive, providing a definition based on what has already been seen is convenient: the equilibrium state of a system is one in which its entropy is maximum. In the last decades the study of processes out of equilibrium has been a subject of study of numerous investigations, being the entropy production a very important part to extend thermodynamics to these cases, an introduction to the corresponding formalism will be seen in Chapter 4.

So far, entropy has been introduced as a purely thermodynamic quantity. Now, continuing with this brief historical review, the Boltzmann's entropy (1877) must be introduced:

$$S_B = k_B \ln(W). \tag{1.6}$$

In a Statistical Physics course, basic arguments are given to arrive at this relationship, which allows calculating the entropy of a system for which has been determined: $W :=$ the number of possible microstates corresponding to the macroscopic state of a system (these concepts will be illustrated later with an example later). The well-known Boltzmann constant k_B also appears in the relationship. Actually, this formula is a particular case of the following, the Gibbs entropy:

$$S = -k_B \sum_i p_i \ln(p_i), \tag{1.7}$$

where p_i is the probability of finding the system in the $i-$th microstate. If all states can occur with the same probability (which occurs for energy, volume and number of fixed particles, i.e., in the microcanonical ensemble): $p_i = p = 1/W$, where W is defined same as before. Therefore:

$$\sum_i p_i \ln(p_i) = -\sum_i p_i \ln(W) = -\ln(W)\sum_i p_i, \quad \sum_i p_i = 1 \ \Rightarrow \ \sum_i p_i \ln(p_i) = -\ln(W).$$

With which it is verified that the relation (1.6) is a special case of (1.7).

Before exploring a bit the link between this definition and the thermodynamic entropy that was discussed at the beginning, the historical review will continue. So far, entropy has been considered as a thermodynamic quantity and as a result of statistical mechanics, now, is the time to include quantum mechanics.

They will also be assumed by known basic concepts of quantum mechanics. For now, only there is interest in knowing the concept of "density matrix", through which John von Neumann introduced the following relationship in 1932, which allows determining the entropy of a quantum system described by certain density matrix ρ:

$$S_{vN} = -k_B \operatorname{Tr}\{\rho \ \ln(\rho)\}. \tag{1.8}$$

Where $\text{Tr}\{A\}$ is the trace over the matrix A. Although the interpretation of this relation is still controversial today [SH06, She99], in what follows it will be used as a result with a clear and precise meaning. It is easy to see that, if the density matrix is written in its eigenbasis, that is, obtaining the base for which $\rho = \sum_i q_i \,|\varphi_i\rangle \langle\varphi_i|$, it will be obtained:

$$S_{vN} = -k_B \sum_i q_i \, \ln(q_i). \tag{1.9}$$

Although the equation (1.7) and the previous one are defined in completely different contexts (statistical mechanics and quantum mechanics), it is clear that they are completely analogous.

The last author to be mentioned in this review will be Claude Shannon, whose contributions were in the field of information theory. In 1948 he obtained a formula for the entropy of *information* of a certain random variable X with a probability distribution with outcomes P_i [Sha48]:

$$S_{Sh} = -K \sum_i P_i \, \log_2(P_i). \tag{1.10}$$

For a certain constant K. It can be seen why in such a different context entropy is also spoken of, again a relation appears in the form of (1.7). The base of the logarithm has changed, it is now base 2, however, this formula can be written with the natural logarithm (in base 2 each entropy unit is referred to as a "bit" and in base e as "nat").

Although the theory behind this relationship is really interesting, it is found in a different context, so it will not be discussed, by the moment. And, since this is not normally learned in a physics grade, it will be reviewed in Chapter 2. For now, it is enough to know that entropy also manifests itself in the context of information theory and it is related with its purely physical meaning.

1.2 A FIRST CLASSICAL EXAMPLE

As mentioned above, there is a relationship between the equation for entropy in statistical terms and thermodynamic entropy, in fact they can be said to be the same thing. However, the general proof of (1.6) remains vague in most statistical mechanics textbooks. But, for example, in [CK10] a worthy derivation can be read. Here, basic knowledge will be used to see, in a particular case, how the thermodynamic entropy can emerge from the relation (1.6), this particular case will be the Joule expansion.

n moles of an ideal gas are considered. For this system, an expression for the entropy change can be determined. The following basic thermodynamic expressions are known:

$$\left(\frac{\partial S}{\partial V}\right)_{T,n} = \left(\frac{\partial P}{\partial T}\right)_{V,n}, \quad \left(\frac{\partial S}{\partial T}\right)_{V,n} = \frac{nC_V}{T} \quad \begin{array}{c}\text{Ideal} \\ \text{gas}\end{array} \Rightarrow P = \frac{nRT}{V} \Rightarrow \left(\frac{\partial S}{\partial V}\right)_{T,n} = \frac{nR}{V}.$$

Integrating and taking into account that $n = constant$:

$$S(T,V) = \int_{V_0}^{V} \left(\frac{\partial S}{\partial V}\right)_T dV = \int_{V_0}^{V} \frac{nR}{V} dV = nR \ln\left(\frac{V}{V_0}\right) + c(T) \Rightarrow \frac{d}{dT}c(T) = \frac{nC_V}{T} \Rightarrow$$

$$\Rightarrow\; S(T,V) = nR\ln\left(\frac{V}{V_0}\right) + nC_V\ln\left(\frac{T}{T_0}\right). \tag{1.11}$$

The ideal gas at temperature T_i is considered enclosed in an initial volume V_i, then another empty container of equal volume is connected, so that the gas expands to $2V_i$. Since the process is adiabatic and there is no work done, the temperature remains constant and, also, it will be obtained that the expression (1.11) will coincide with the entropy production during the expansion. Finally:

$$S(T,V) = nRT\ln\left(\frac{2V_i}{V_i}\right) + nC_V\ln\left(\frac{T_i}{T_i}\right) = nR\ln(2). \tag{1.12}$$

So far, the calculations have been purely thermodynamic, no statistical or quantum mechanics was involved. But, now, the expression (1.6) is considered. And it is only necessary to know W, which can be obtained by a fairly simple probabilistic reasoning.

Each gas molecule can now be found in the initial container or in the container that has been connected, then, there are two possible containers for each molecule. In other words, the process adds an uncertainty to the state of the system, stemming from the ignorance of the container in which each molecule is located. In fact, this can be taken as an interpretation of the entropy production in the system (this will be evident after Chapter 2). Thus, it is clear that the total number of possibilities, taking into account that there are $N = n \cdot N_A$ molecules and ignoring considerations regarding the distinguishability of the molecules, will be 2^N. With which, the entropy production in the process is:

$$S_B = k_B\ln(W) = k_B\ln\left(2^{n\cdot N_A}\right) = nN_Ak_B\ln(2) = nR\ln(2). \tag{1.13}$$

Where it has been used that $k_B N_A = R$. As it can be seen, the two expressions for the entropy variation coincide, (1.13) $\equiv$ (1.12). This is a beautiful example of how thermodynamic entropy can emerge from a purely statistical relation, and it is also a way to give an interpretation in statistical terms to the entropy production. It has also served to illustrate a typical calculation of microstates corresponding to a macroscopic state of a system.

1.3 One application and motivation

As mentioned at the beginning, thermodynamics arose from the need to study steam engines. And now the goal is almost the same: one of the main applications of quantum thermodynamics is the study of heat engines. As is well known, Carnot made very important contributions to the analytical study of heat engines and his developments can be condensed into his famous theorem:

All heat engines between two heat reservoirs at temperatures T_C and T_H $(T_H > T_C)$ are less efficient than a Carnot heat engine operating between the same reservoirs.

$$\text{Being the Carnot's efficiency equal to }\;\; \eta_c = 1 - \frac{T_C}{T_H}. \tag{1.14}$$

Previously it was mentioned that entropy production can characterize how irreversible a process is, with the previous statement this is clear, but first it will be necessary to

express it in a somewhat different way. The objective, first, will be to write the first and second laws of thermodynamics in terms of rates (time derivatives). In this way, the previous statement of Carnot's theorem and the statement of the second principle by Clausius and that of Kelvin-Planck can be recovered, but only the first one will be seen here, in [LP20] all the implications of writing these principles in terms of time derivatives can be reviewed.

From the typical expressions of the first principle and the second principle (equation (1.4)), for a system interacting with two reservoirs (H and C with $T_H > T_C$), it is obtained:

$$\left.\begin{array}{l} 1^{st} \text{ Principle}: \Delta U = W - Q = W - Q_H - Q_C \\ 2^{nd} \text{ Principle}: \Sigma = \Delta S + \frac{Q_H}{T_H} + \frac{Q_C}{T_C} \end{array}\right\} \Rightarrow \left.\begin{array}{l} \frac{d}{dt}U = \dot{W} - \dot{Q} = \dot{W} - \dot{Q}_H - \dot{Q}_C \\ \dot{\Sigma} = \frac{d}{dt}S + \frac{\dot{Q}_H}{T_H} + \frac{\dot{Q}_C}{T_C} \end{array}\right\}$$

There it was taken $Q > 0$ when it leaves the system and $W > 0$ for work pulled from the system (energy leaves it).

For a long enough time, all the work done will be the result of the heat exchanged, and the entropy of the system will be constant. That is, a steady-state will be reached, which is characterized by the temporal invariance of the variables that characterize the system (state variables), which in this case are energy and entropy (obviously the entropy production, heat and work are not state variables). When the cycle reaches this point, it is called a limit cycle.

On the other hand, the efficiency of the system doing work can be defined as $\eta = \dot{W}/\dot{Q}_H$. If the system has reached a steady-state, the following can be written:

$$\dot{W} = \dot{Q}_H + \dot{Q}_C \quad \& \quad \dot{\Sigma} = \frac{\dot{Q}_H}{T_H} + \frac{\dot{Q}_C}{T_C} \Rightarrow \eta = 1 - \frac{T_C}{T_H} + \frac{T_C}{\dot{Q}_H}\dot{\Sigma} = \eta_c + \frac{T_C}{\dot{Q}_H}\dot{\Sigma}. \quad (1.15)$$

With the previous relation it is clear that the entropy production quantifies how far a certain engine deviates from doing work with the maximum efficiency (Carnot efficiency). Specifically, when the process that the system undergoes is irreversible, the efficiency will be reduced above the maximum by the amount $T_C\dot{\Sigma}/\dot{Q}_H$.

Note 1: classical entropy is defined for a state of equilibrium, so, strictly speaking, it is being assumed that the system is in a state of equilibrium at every instant.

Note 2: the quantity $T_C\dot{\Sigma}/\dot{Q}_H$ is always less than 0, as it must be to ensure that $\eta \leq 1$. This is because $\dot{Q}_H < 0$ (the hot reservoir brings heat to the system), naturally $T_C > 0$ and aldo $\dot{\Sigma} > 0$. The latter is a way of writing the second principle and is obtained from the relation (1.5) and assuming $dt > 0$.

All of the above is useful as a review of the most basic knowledge about entropy in different contexts of physics. In addition, the importance of the study of processes through the entropy production formalism has become clear, which justifies the interest in related research and is the motivation for this work.

So, the next goal will be to try to understand entropy in a broad sense, so that it is possible to address the complexity involved in the study of quantum systems, which will be seen in Chapter 3. For this, as mentioned above, the knowledge presented in Chapter 2 is needed. Finally, as noted in the historical remarks, fluctuation theorems will be reviewed in Chapter 4, as they are an important part of current research.

All in all, that's the scope of this work.

CHAPTER 2

INFORMATION THEORY AND THERMODYNAMICS

Resumen

La conexión entre la teoría de la información y la termodinámica es algo que no surgió hace demasiado, hasta hace solo unas cuantas décadas había importantes problemas abiertos, uno de ellos se comenta en la última sección de este capítulo. Por esto, aquí se dará una base de conocimientos de teoría de la información, haciendo hincapié en definiciones importantes para desarrollos posteriores. También se trata de dar una intuición de la conexión que hay entre la teoría de la información y la termodinámica, ilustrando las ideas con ejemplos. Como resultado, se tendrán las herramientas para dar una interpretación básica de la entropía en cualquier contexto.

2.1 BASICS ABOUT INFORMATION THEORY

At the moment, entropy is known with total clarity as a purely thermodynamic quantity, but very little has been said about its interpretation in the context of information theory. In order to clarify this, it will be tried to give meaning to the Shannon entropy relation, (1.10). And having this base will be necessary to establish the link between the two contexts and to be able to understand the results of the next chapters.

It has not yet been precisely defined what *information* is in the context of information theory, that is, the one mentioned before writing (1.10) in Section 1.1. To do this, a certain random variable X with a probability distribution with outcomes P_i is considered. Then, the information associated with the event n (an event can be understood as a measurement), with the result x_n and whose probability is P_n, is usually defined as:

$$I(x_n) = -\log_2(P_n). \tag{2.1}$$

It is common to find this definition in the literature, like in [Wil11]. The previous formula can be interpreted as a measure of the "surprise" of having obtained the value x_n after the event n or, what is the same, the "uncertainty" before the value x_n is obtained.

For example, 100 balls are kept in a box. First, it will be assumed that they are all the same color, it is evident that the probability of finding a black ball when taking one

out of the box (this would be the event or measurement) will be $P_{black} = 1$, therefore, $I(black) = -\log_2(1) = 0$. That is, the surprise is zero, which coincides with what was expected because it was already known that the ball that had been taken would be black. And what would happen for a ball of another color? For any other color, for example white, the probability is 0, with which $I(white) = -\log_2(0) \to \infty$. Knowing that all balls are black, the surprise of finding a white one would be immeasurable. Both the numerical result and the assumption itself are absurd and, again, the relationship is true.

Similarly, now it is considered that there are 99 black balls and one white, the information for each result will be $I(black) \simeq 0.014$ and $I(white) \simeq 6.644$. Again, results are consistent with expectations, great surprise for the least probable result and little for the most probable result. This, together with the previous example, shows the intention of defining the information as in (2.1).

This quantity only gives information about one outcome of the random variable X. It is natural to aim to get an overview of the surprise that is contained in the entire random variable X. And one way to get that insight can be to calculate the information for any possible outcome and average each one, using the probabilities of each outcome as weights. In [Wil11] this average is called "expected information content" and takes the form:

$$H(X) = \sum_n P_n I(x_n) = -\sum_n P_n \log_2(P_n). \tag{2.2}$$

In fact, this is the definition of entropy in information theory and except for a constant factor, it is the same expression as (1.10). It should be noted that in this definition and in the other occasions in which something of the form $a \log_b(a)$ appears, for the case in which $a = 0$ it is taken $0 \log_b(0) = 0$, this not only makes sense mathematically (it is clear that $\lim_{a \to 0} a \log_b(a) = 0$), it is also clear that it would be absurd to consider a result that is not possible, as in the example of the 100 black balls.

As with the equation for information, an example can be developed in order to settle the specific meaning of the above relationship. A certain 4-letter alphabet is assumed: A, B, C and D. Each can be found in a text made with that alphabet with probabilities $1/2, 1/4, 1/8$ and $1/8$, respectively. These probabilities form a probability distribution with a random variable that will be denoted as Z. It is possible to calculate its entropy:

$$H(Z) = -\frac{1}{2} \log_2\left(\frac{1}{2}\right) - \frac{1}{4} \log_2\left(\frac{1}{4}\right) - \frac{1}{8} \log_2\left(\frac{1}{8}\right) - \frac{1}{8} \log_2\left(\frac{1}{8}\right) = \frac{7}{4} = 1.75.$$

On a computer each letter can be encoded as a number, for example $A \equiv 00, B \equiv 01, C \equiv 10$ and $D \equiv 11$. Thus, each one is said to have 2 bits. A question arises: taking into account the probability of finding each letter, what is the best way to encode them? And the best way is considered to be the one for which fewer bits are used, on average.

In [Sha48] Shannon showed that: it is not possible to encode the outcomes of a random variable X with fewer than $H(X)$ bits, on average. This is called "the source coding theorem". Also, the appropriate number of bits to encode each result x_i with probability P_i will be $\log_2(1/P_i)$. Going back to the example, this would correspond to:

	Bits	Code
A	1	0
B	2	10
C	3	100
D	3	010

The choice of the code for each letter in this table is arbitrary, only the necessary number of bits is respected. And, in effect, it is obtained that the average number of bits needed is, weighting with each probability, $1/2 \cdot 1 + 1/4 \cdot 2 + 1/8 \cdot 3 + 1/8 \cdot 3 = 1.75$, which is the entropy calculated above.

It should be taken into account that the fact of being able to use more or less bits, on average, is a consequence of the fact that it is possible to take advantage of the fact that it is known that each letter will appear with a certain probability.

In short, it can be said that the definition of Shannon's entropy, (2.2) or (1.10), takes on a very intuitive and justified meaning through the source coding theorem.

2.2 The link between Shannon entropy and thermodynamic entropy

Once the foundations of entropy have been laid in the context of information theory and statistics, it is possible to establish a relationship between them. There are many ways to start the argument, but the reasoning detailed in [Sch19] will be followed here.

Actually, everything that is necessary to establish the link is already there, which was to be expected considering that the relation (2.2) and the (1.7) are completely analogous. It is enough to *interpret that the microstates, with probabilities p_i, correspond to the data in the context of Shannon entropy*. In the example of the alphabet with A, B, C and D, each of these letters would be a possible microstate of a physical system.

Note: entropy is usually interpreted in statistics as *disorder*, but now a more general interpretation can be given. The interpretation given in the previous section, in short, is that of *measure of uncertainty* that the system has or, what is the same, *the lack of information* that someone has about the system. And this will be the interpretation that will be given to it in the rest of the areas.

It would be of great interest to have a relation that connects information theory with classical thermodynamics. And a typical example is Landauer's principle. Before stating this important principle, the idea behind it will be illustrated with a common case in computer physics.

A system like the one shown in Figure 2.1a is considered, i.e., a particle (considered classical) in a bistable potential well. Each well corresponds to a digit, a 0 or a 1, this is a simple system to model how information is stored in a computer, in this way the information of a letter in the example of the alphabet could be stored. That is, this is a system capable of store a bit of information. It has been chosen that the two wells are equally deep since in this way there is no a privileged one, so 0 and 1 can be assigned arbitrarily, just like when coding a letter in the previous examples.

Now it can be considered a typical operation on the system, for example: "restore to 0". That is, if the particle is in state 0, after the operation it will remain in that state and, if the particle is in state 1, after the operation it will be in state 0. An important question can be raised: what is the minimum energy required to perform the operation?
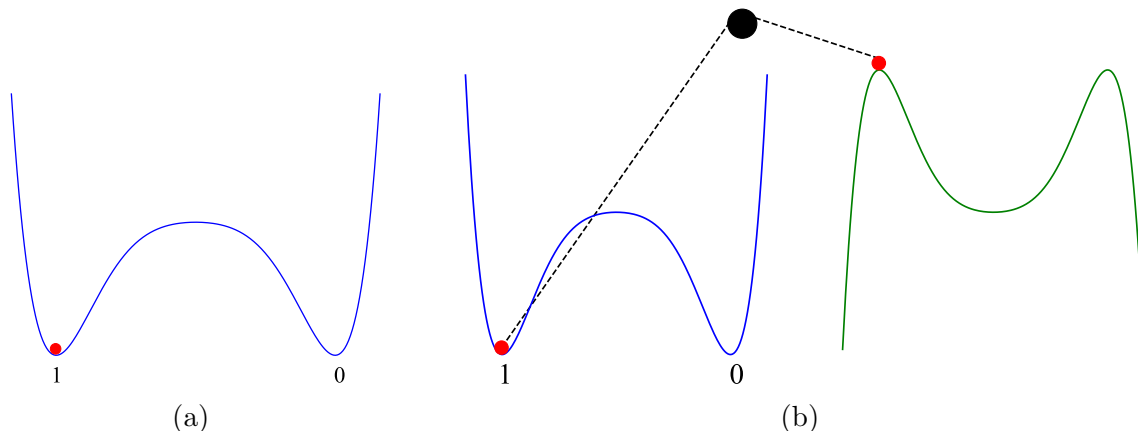
Figure 2.1: (a): bistable potential well. (b): bistable potential well with possible a system so as not to need energy during the operation.

The system in Figure 2.1b shows how a potential opposite to the given one can be used to avoid having to invest energy in the operation. It is prepared so that, when the particle is at a minimum, the other is at a maximum, that other is linked to the first by a string, so that changing the particle from state 1 to 0 does not require energy. Thus, at first sight it seems possible to perform the operation without any expenditure of energy. But, in that way, two different routines are used, depending on the initial state of the device (0 or 1). But this is not how computers work, so, is it possible to construct a *single* time-varying force, $F(t)$, to perform the operation without energy loss? Here, "single" means that a process with two different routines is avoided.

In [Lan00] this question is solved in a very elegant way: the force $F(t)$ is not a bijective function (specifically, it is not injective) by construction, so it is not a physically possible force. And this is because the laws of mechanics are time-reversible, then, all related functions must be reversible, i.e., bijective. But $F(t)$ applied in state 0 or state 1 gives the same result, so it is not injective, that is, it cannot be time-reversible.

But if it is assumed that there is loss of energy, it is possible to construct a single time-varying force, for example, if some kind of "friction" is added to the potential. If a force (given by $F(t)$ and regulated correctly) is applied at the position of 1 but the particle is at 0, the operation is carried out correctly, the particle ends up at 0. And if the force is applied at 1 when the particle is there, it will go over the hill, reach 0 and due to friction it will lose energy until it is static at 0, also in this case the operation is carried out. Here, that friction is absolutely essential, since without it the particle would go up the potential "wall" and, after that, would have enough energy to return to 1, so the operation would not be executed.

Now it is important to observe the following: after the operation, whatever the way to carry it out, one bit of information has been erased, because after that it is not possible to know in what state the particle was initially. On the other hand, it should be noted that with the previous development it has finally been possible to talk about concepts of information theory (the information bit) together with thermodynamic concepts (dissipation of energy). And it turns out that the above statement about erasing information is a

well known physical principle, that is Landauer's Principle:

> Erasing information requires energy be dissipated as heat, so the entropy in the environment to which the information storing system is connected must increase

The link with entropy can be seen through, for example, the equation (1.4), in which heat and entropy appear related. Specifically, it can be obtained by a more or less simple procedure, such as the one detailed in [Jac05], that the minimum possible amount of energy and the corresponding increase in entropy required to erase one bit of information are:

$$E = Tk_B \ln(2) \qquad (2.3a) \qquad S = k_B \ln(2). \qquad (2.3b)$$

Where T is the temperature of the sink where heat is entering after bit erasing.

In conclusion and returning to the main topic of this work, it can be stated that the erasure of a bit of information entails a minimum entropy production, given by the previous relation. In addition, an interpretation about entropy production, in the information theory framework, can already be given: *the entropy production is a way to know how much information about a system is erased (is no longer accessible) during a process.*
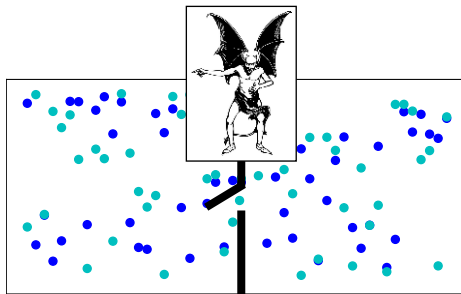
Note 1: the previous results are valid for systems of an arbitrary dimension, since the Landauer's Principle does not place restrictions on the size of the systems. So, despite not having explicitly talked about quantum systems, the previous results could be applied to microscopic systems.

Note 2: actually, the laws of physics are still reversible in the case of the double well with friction, in principle anyone could know where the particle was initially. But this would require information about all the particles that have carried heat, which is not accessible. It is really in this ignorance of the rest of the particles involved where the bit of information has been erased.

2.3 MAXWELL'S DEMON

An application of all the above formalism is found in the resolution of the paradox of the Maxwell's Demon. In 1867, James Clerk Maxwell proposed a thought experiment like the one shown in Figure 2.2 (will be explained below) and about which too much has been written since then, as the involved paradox caused problems during about 100 years. In [Hil14] can be found a detailed discussion and many details about it, although in [Fey96, Sch19] there are more concise developments (those that will be given here).

A certain element gas is considered confined in a box, which is divided into two vessels. This gas has its molecules in motion and, according to a certain

Figure 2.2: Maxwell's demon letting a cold particle go to the left.

criterion, these are classified as "slow" and as "fast", in Figure 2.2 the slow ones are shown in light blue and the fast ones in blue. One possibility would be to consider that all those

that go with a lower speed than a certain speed v will be slow and those that have a higher speed will be fast. Now, somehow, the fast molecules are separated by putting the fast ones in one vessel and the slow ones in the other. For example, a small demon can be put in the box. And this demon opens a door or closes it if a molecule approaches, so that if it is slow it goes to the left or, if it was already on that side, it stays there. After carrying out this operation, the demon observes another molecule. And analogously for the fast molecules.

It should be noted that there are other ways of setting up the experiment, for example in [Sch19] two mixed (different) gases are considered and they are divided in the vessels according to each gas.

After enough time, that activity will have separated the hot (fast molecules) from the cold (slow molecules), creating a temperature difference between the two sides of the box. This goes against the Kelvin-Planck statement of the second principle of thermodynamics, since work could be extracted from the temperature difference between the two sides with no other effect (it is clear that moving the door can be done without energy cost).

This is equivalent to saying that the entropy of the system (the gas inside the box) decreases, which goes against (1.5), since this is also an isolated system. The important thing is that there is a contradiction to the second principle, hence the paradox. The resolution of this problem took more than 100 years, so here only an intuitive idea will be given, presented in [Ben81], but also a somewhat different perspective is posed.

It turns out that the process carried out by the demon entails an erasure of information. Initially, the demon will be in a state of uncertainty S, and it must observe whether a molecule (one that it decides to look at) is moving to the left or to the right and its velocity. If it moves to the left, the state of the demon will become L and, if it moves to the right, the state will become R. But for the next measure, it will be necessary to put the demon back in its uncertain state S, so it is necessary to erase the information of the previous state. And this carries an energy cost, which at least will be given by (2.3a). In the end it will be obtained that, by erasing information, the energy required to put all the slow molecules on one side will be equal to the work that can be extracted from the system due to the temperature difference. So the second principle is not being broken.

With the same objective, a new approach to resolution will now be proposed, but it is really something equivalent. The number 0 can be assigned to the left side of the box and 1 to the right, as described in the previous section. The action of setting the slow molecules to 0 is equivalent to doing the restore to 0 operation. That is, if the initial state of the slow molecule is 0 (it is on the left side), let it continue like this, and if the initial state is 1 (it is on the right side), let it go to 0. In either case, the information on the side the molecule was initially on is being lost (erased). Hence the cost of energy that compensates for the work that can be extracted.

In conclusion and, connecting with the main topic, it has turned out that *the erasure of information and the corresponding entropy production are the key to the resolution of the paradox*, obtaining that $\Sigma = 0$ for the total system (the gas, the demon and the environment), in good agreement with (1.5). Actually, if the information deletion is not optimal, then $\Sigma > 0$, it entails greater entropy production. This problem prompted the aforementioned authors Charles Bennett and Rolf Landauer to their results on information and entropy, hence its importance.

CHAPTER 3

STUDIES IN QUANTUM SYSTEMS

Resumen

La relevancia del estudio de la entropía y, más concretamente, de la producción de entropía en sistemas cuánticos está clara. Por lo que es de interés buscar una relación que permita hacer cálculos de esta cantidad. Se han hecho muchos trabajos al respecto, pero en este capítulo se demuestra una relación concreta para determinar la producción de entropía en un sistema que se pone en contacto con un entorno, lo cual es una situación muy típica, de ahí el interés por esa fórmula. Además, se aplica esta a dos modelos concretos, con lo que se comprueba su utilidad y eficacia.

3.1 QUANTUM ENTROPY

In all of the above, a classical statistical and thermodynamic interpretation of entropy has been given. However, as already mentioned in Section 1.1, the entropy of a quantum system given by the relation (1.9) is in perfect agreement with the definition of Gibbs entropy (statistics). It was also initially mentioned that this equation, whose general form is the von Neumann equation, (1.8), is still controversial. So its obtaining will not be detailed.

However, it can be seen that it makes sense to define the entropy of a quantum system in this way. A system that is in a pure state $|\psi\rangle$ is assumed, therefore, its density matrix will be $\rho = |\psi\rangle\langle\psi|$. So, according to (1.8), the entropy of the system is $S = -k_B \cdot 1\ln(1) = 0$. But if the system is in a mixed state like $\rho = \frac{1}{2}|\psi_1\rangle\langle\psi_1| + \frac{1}{4}|\psi_2\rangle\langle\psi_2| + \frac{1}{4}|\psi_3\rangle\langle\psi_3|$, the entropy will be $S = -k_B\left(\frac{1}{2}\ln\left(\frac{1}{2}\right) + \frac{1}{4}\ln\left(\frac{1}{4}\right) + \frac{1}{4}\ln\left(\frac{1}{4}\right)\right) = k_B\ln(8)/2 \neq 0$.

In the first case, by hypothesis, the quantum state of the system is certain, there is no *uncertainty*. But in the second there is a lack of knowledge of the state in which it can be found. Indeed, for the case with uncertainty, an entropy different from 0 appears, in good agreement with the accepted interpretation for entropy, given previously. Ultimately, the quantum states in which the system can be found are equivalent to the A, B, C and D from the alphabet example in Section 2.1.

It should be noted that, as is evident, for the calculation of entropy only the probabilities corresponding to the components of the statistical mixture appear. The probabilities obtained from the measurement of an observable do not come into play, that is, the purely quantum probabilities. However, an entropy based on quantum probabilities can also be

defined, which is different from 0 also for pure states. One example is called "operator entropy" and it quantifies the amount of information about some property (given by an certain operator) that is missing in the quantum state. The von Neumann entropy can be seen as a special case of quantum operator entropy when the operator is the density matrix, [Len19]. However, only the von Neumann entropy will be considered, at least now.

In words of O. Shenker, who has criticized the validity of von Neumann entropy: "von Neumann entropy characterizes the quantum probabilistic properties of a system. This characterization is useful, leading to successful and important predictions", [She99]. Ultimately, the expression (1.8) will be accepted as the expression for the entropy of a quantum system without further discussion or more developments.

3.2 ENTROPY PRODUCTION

This is a fundamental part of this work and, unfortunately, the first thing to say is that *there is no general formulation for entropy production in quantum systems* [LP20, ELVdB10]. In the following, where is the problem will be seen.

A system with Hamiltonian H_s It is considered and is assumed to be described at time $t = 0$ by a density matrix $\rho_s(0)$. Therefore, according to the well-known Liouville-von Neumann equation and assuming time-independent hamiltonians, the state of the system at time t can be determined by the following:

$$i\hbar \frac{\partial \rho_s}{\partial t} = [H_s, \rho_s] \quad (3.1a) \quad \Rightarrow \quad \rho_s(t) = U\rho_s(0)U^\dagger \ \text{ with } \ U = \exp\{-iH_s t/\hbar\} \quad (3.1b)$$

The above is a unitary transformation, that is: $UU^\dagger = \mathbb{1}$, where $\mathbb{1}$ is the identity operator. And it is well known that *von Neumann entropy is constant under unitary evolution*, i.e., $S_{vN}(\rho(0)) = S_{vN}(\rho(t))$. If this system is considered to be the entire universe, the entropy production between the instants 0 and t will be $\Delta S = S_{vN}(\rho(t)) - S_{vN}(\rho(0)) = 0$, or what is the same, $\Sigma = 0$. But in this case, where does irreversibility emerge in any physical process? This is not a trivial problem. It turns out that, in most cases in the study of a quantum system, it is necessary to introduce irreversibility particularizing for each case and using the corresponding approximations.

3.2.1 OBTAINING A USEFUL AND TYPICAL FORMULA

In [ELVdB10] a relation for the entropy production that is useful in many situations is proposed. The idea given there is to consider that the total system is a concrete system S in contact with a set of environments $E_1, E_2, E_3 \ldots$ that are heat reservoirs. The evolution of the total system is considered to be given by (3.1b), but the objective is to determine the entropy production in S, which will not be constant.

It is also considered that each environment is in a canonical equilibrium state at temperature T_i (with $i = 1, 2, 3 \ldots, n$) at time $t = 0$, i.e., if the hamiltonian of the corresponding environment is H_i, the density matrix that characterizes this part of the total system will

be given by:

$$\rho_i = \frac{\exp\{-H_i\beta_i\}}{\mathcal{Z}_i} \quad \text{with} \quad \beta_i = \frac{1}{k_B T_i}, \tag{3.2}$$

where $\mathcal{Z}_i$ (the partition function) is necessary to ensure $\text{Tr}\{\rho\} = 1$. It is also assumed that, initially, the total system can be written as the following tensor product:

$$\rho(0) = \rho_S(0) \otimes \rho_1(0) \otimes \cdots \otimes \rho_n(0). \tag{3.3}$$

When the density matrix of a system that has two parts can be written in this way, it is said that there are no correlations between the corresponding subsystems.

Finally, the hamiltonian of the total system is considered to be:

$$\text{sum of subsystems hamiltonians and the interaction: } H = H_s + \sum_{i=1}^{n} H_i + V. \tag{3.4}$$

As it was noted above, the goal now is to determine the entropy production of the system S. But, for that, it is necessary to know the state of the system at any instant of time, this can be obtained from the density matrix of the total system at any time, $\rho(t)$, and that is:

$$\rho_S(t) = \text{Tr}_{Es}\{\rho(t)\}. \tag{3.5}$$

Where $\text{Tr}_{Es}\{A\}$ denotes the partial trace of the A operator over the degrees of freedom of the environments. And $\rho(t)$ is obtained analogously to (3.1b) but with (3.4).

The authors of [ELVdB10] already show the developments until reaching the final formula, but a little more detail will be given here. It is important to say that all the properties that will be mentioned can be found in [NC11].

First, the fact that the entropy of the total system remains constant will be used. And, taking into account the property for which $S_{vN}(\rho_1 \otimes \rho_2) = S_{vN}(\rho_1) + S_{vN}(\rho_2)$ (**Property 1**), the following will be reached:

$$-\text{Tr}\{\rho(t)\ln(\rho(t))\} = -\text{Tr}\{\rho(0)\ln(\rho(0))\} = -\text{Tr}\{\rho_S(0)\ln(\rho_S(0))\} - \sum_{i=1}^{n}\text{Tr}\{\rho_i(0)\ln(\rho_i(0))\} \Rightarrow$$

$$\Rightarrow \text{Tr}\{\rho_S(0)\ln(\rho_S(0))\} = \text{Tr}\{\rho(t)\ln(\rho(t))\} - \sum_{i=1}^{n}\text{Tr}\{\rho_i(0)\ln(\rho_i(0))\}.$$

The entropy change in the system will then be:

$$\Delta S_{vN}(\rho_S) = S_{vN}(\rho_S(t)) - S_{vN}(\rho_S(0)) =$$

$$= \text{Tr}\{\rho_S(t)\ln(\rho_S(t))\} + \text{Tr}\{\rho(t)\ln(\rho(t))\} - \sum_{i=1}^{n}\text{Tr}\{\rho_i(0)\ln(\rho_i(0))\}.$$

On the other hand, there is an important property by which, for a system with two parts A and B with a density matrix ρ_{AB} (there may be correlations) it is true that $\text{Tr}\{\rho_{AB}\ln(\mathbb{1}_A \otimes \rho_B)\} = \text{Tr}\{\rho_B\ln(\rho_B)\}$ (**Property 2**), where $\mathbb{1}_A$ is the unity operator in Hilbert space of subsystem A. Thus, eliminating the identity operator from the notation, is obtained: $\text{Tr}\{\rho_S(t)\ln(\rho_S(t))\} = \text{Tr}\{\rho(t)\ln(\rho_S(t))\}$. Combining that property

with another one for which $\mathrm{Tr}\{\rho(t)\ln(\rho(t))\} = \mathrm{Tr}\{\rho(t)\ln(\rho_S(t) \otimes \rho_1(0) \otimes \cdots \otimes \rho_n(0))\} + \sum_i \mathrm{Tr}\{\rho_i(t)\ln(\rho_i(0))\}$ (**Property 3**), after a straightforward manipulation, the next relation is obtained:

$$\Delta S_{vN}(\rho_S) = -\mathrm{Tr}\{\rho(t)\ln(\rho_s(t) \otimes \rho_1(0)) \otimes \cdots \otimes \rho_n(0))\} + \mathrm{Tr}\{\rho(t)\ln(\rho(t))\} +$$
$$+ \sum_{i=1}^{n} \mathrm{Tr}\{(\rho_i(t) - \rho_i(0))\ln(\rho_i(0))\}. \tag{3.6}$$

The last term of the previous relation can be developed a little more considering that it is of the form (3.2):

$$\sum_{i=1}^{n} \mathrm{Tr}\{(\rho_i(t) - \rho_i(0))\ln(\rho_i(0))\} = \sum_{i=1}^{n} \beta_i \, \mathrm{Tr}\left\{H_i\left(\rho_i(0) - \rho_i(t)\right)\right\}.$$

By the very definition of the density operator, the mean value of H_i will be $\mathrm{Tr}\{H_i\rho_i\}$, which is the energy of the system i. Therefore, $\mathrm{Tr}\left\{H_i\left(\rho_i(0) - \rho_i(t)\right)\right\}$ gives the energy variation in the environments, but with a changed sign, so it could be interpreted as *the heat entering the system S* which will be denoted as $Q_i = \mathrm{Tr}\left\{H_i\left(\rho_i(0) - \rho_i(t)\right)\right\}$.

On the other hand, for the other term, it is convenient to introduce the definition of relative entropy. The relative entropy of the density matrix σ_1 with σ_2 is defined as:

$$S(\sigma_1||\sigma_2) = \mathrm{Tr}\{\sigma_1\ln(\sigma_1)\} - \mathrm{Tr}\{\sigma_1\ln(\sigma_2)\}. \tag{3.7}$$

Therefore, for the remaining terms of the relation (3.6):

$$-\mathrm{Tr}\{\rho(t)\ln(\rho_s(t) \otimes \rho_1(0)) \otimes \cdots \otimes \rho_n(0))\} + \mathrm{Tr}\{\rho(t)\ln(\rho(t))\} =$$
$$= S(\rho(t)||\rho_s(t) \otimes \rho_1(0) \otimes \cdots \otimes \rho_n(0)).$$

By definition, it is true that $S(\sigma_1||\sigma_2) \geq 0$, so it is a quantity that in any case entails an increase in entropy. This was a necessary requirement to have a consistent definition of entropy production, as shown in equation (1.5). It will be justified more rigorously later, but it turns out that from the above is obtained the definition that was tried to be found for the entropy production in a quantum system under the conditions described above. Hence, for the system S the entropy production is:

$$\boxed{\Sigma = S\left(\rho(t)||\rho_s(t) \otimes \rho_1(0) \otimes \cdots \otimes \rho_n(0)\right)} \tag{3.8}$$

And, therefore, for the entropy variation of the system it remains:

$$\Delta S_{vN}(\rho_S) = \sum_{i=1}^{n} \beta_i Q_i + \Sigma \tag{3.9}$$

With the definitions that have been made previously, this has resulted, which is in perfect agreement with (1.4). Of course, that the previous result has an analog in the context of classical thermodynamics is a very good sign and gives a physical basis to the previous

result. However, a clearer interpretation of the expression for Σ above will be given in the next section.

Note: Normally, master equations are used to know the evolution of a system in contact with an environment, the Liouville-von Neumann equation is not usually used. But for a calculation of entropy production, as has just been seen for this procedure, it is necessary to know the density matrix of the environment, which cannot be achieved with master equations, that are obtained from approximations that are not suitable here.

3.2.2 Interpreting formula (3.8)

There are many ways to see that (3.8) makes sense as a proposal for calculating entropy production in a quantum system. Many authors have contributed with their vision of this relationship, for example in [LP20, ELVdB10] is justified from various points of view. Some of these most basic ideas will be condensed here, specifically, two interpretations are given:

Interpretation with relative entropy

Relative entropy was defined in (3.7) and, intuitively, it is always defined as a "distance" (it is not a proper distance) between the density matrices σ_1 and σ_2. For example, if $\sigma_1 = \sigma_2$ the value of the relative entropy is 0, the distance between those two matrices is 0 because they are the same. In a classical context it is also defined in a similar way, specifically, for two probability distributions P and Q on the same index set, x, the relative entropy of P to Q is defined as the following:

$$H(P||Q) = \sum_i p_i \ln \left(\frac{p_i}{q_i} \right).$$

This is a measure of how similar the P and Q distributions are. P is considered a reference distribution, while Q usually occupies the role of a distribution obtained by some model that is to be compared with the real data.

Therefore, in (3.8) the matrix $\rho(t)$ is being compared with $\rho_s(t) \otimes \rho_1(0) \otimes \cdots \otimes \rho_n(0)$, which has a very specific physical meaning that is explained below.

At time t the state of the system S is known because it has been traced on the degrees of freedom of the environments, but in this way information is being lost, since when making the partial trace (relation (3.5)) elements of the $\rho(t)$ matrix are being discarded. But how much information has been lost? It would be necessary to compare with the total matrix $\rho(t)$, and to make a quantitative calculation the relative entropy can be used, with which the relation for Σ is justified. In short, (3.8) gives a measure of how much information is lost when tracing to obtain the state S, which is equivalent to giving a measure of how much the uncertainty has increased, in good agreement with the physical definition of the entropy production.

Connecting with the example of Section 2.2 of the particle in the bistable well with "friction", the system S would be the particle that is in 1 or in 0 and the environments would be modeling particles from the walls of the well, in which the energy of the particle is dissipated by friction.

Interpretation with relative entropy and mutual information

First, it is necessary to define mutual information. Let X and Y be two random variables with probability distributions P_x, P_y and with joint distribution P_{xy}, then, the mutual information between X and Y is:

$$H(X;Y) = H(X) + H(Y) - H(XY).$$

Where $H(X)$ and $H(Y)$ are the entropies of each variable (relation (2.2)) and $H(XY)$ the joint entropy obtained from P_{xy}. This amount measures how much information X and Y have in common. So, only if X and Y are completely independent the mutual information is 0. And an important property of mutual information is that $H(X;Y) \geq 0$.

Previously, the joint distribution of two variables has not been discussed, so that definition can be confusing, but with the quantum equivalent it can be easily understood. The mutual information between the density matrices ρ_{AB}, ρ_A and ρ_B, corresponding to the total system AB and with $\rho_A = \text{Tr}_B\{\rho_{AB}\}$, $\rho_B = \text{Tr}_A\{\rho_{AB}\}$ those of the A and B systems, is given by:

$$\mathcal{I}_{\rho_{AB}}(A:B) = S_{vN}(\rho_A) + S_{vN}(\rho_B) - S_{vN}(\rho_{AB}).$$

Manipulating the relation (3.8) to include the mutual information and using properties that have already been mentioned, is obtained:

$$\Sigma = \mathcal{I}_{\rho(t)}(S:E_1:\cdots:E_n) + \sum_{i=1}^{n} S(\rho_{E_i}(t)||\rho_{E_i}(0)). \tag{3.10}$$

Where $\mathcal{I}_{\rho(t)}(S:E_1:\cdots:E_n) = S_{vN}(\rho_S(0)) + \sum_{i=1}^{n} S_{vN}(\rho_{E_i}(0)) - S_{vN}(\rho(t))$. This can be understood as two separate contributions.

The first term of the above relation gives a measure of how similar the matrix of the total system $\rho(t)$ and the reduced matrices of all systems are, with the environments separately. To physically interpret this term, it must be taken into account that the system and the environments have "shared" information during evolution, since the matrix of the total system is no longer the tensor product od system and environment density matrices because correlations have appeared. Therefore, the mutual information gives a measure of the information that has been lost (erased) by discarding the degrees of freedom of the environments and obtaining the reduced state $\rho_S(t)$.

The second term shows how much the state of each environment has changed with respect to the initial one, for each E_i. That is, the information that is lost if the state of each system E_i cannot be known at time t. This together with the first one gives a good physical interpretation for the entropy production.

3.3 APPLICATION TO PARTICULAR SYSTEMS

This section is of great interest, since here the results of having applied the previous formalism to real physical systems are presented. The results of the previous sections are very general and can be applied to arbitrary systems, but models with physical sense will be chosen to illustrate the concepts.

3.3.1 Jaynes–Cummings model

This model was proposed in 1963 in [JC63] and describes a two-level system interacting with a quantized mode, which is modeled as a harmonic oscillator. The hamiltonian of the total system in this model is written as:

$$H = \frac{\hbar}{2}\omega_a\sigma_z + \hbar\omega_b N + \hbar\frac{\omega_c}{2}(a\sigma_+ + a^\dagger\sigma_-). \tag{3.11}$$

Here σ_z, σ_+ and σ_- are the typical spin operators, defined as usual, N is the number operator, a the annihilation operator and $a^\dagger$ the creation operator. The factors ω_a, ω_b and ω_c are frequencies.

The details about how the above is obtained will not be discussed, it will be enough to know that the first term corresponds to the hamiltonian of the two-level system, the second is the hamiltonian of the quantized mode and the last two terms correspond to the interaction between the two systems.

What was done with this model was, first, numerically solve the Liouville-von Neumann equation, (3.1). But to do that it is necessary to set the initial state for the total system. First, a non correlated state was chosen, a tensor product of the state of the system with that of the quantized mode:

$$\rho_S(0) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \qquad \rho_{qm}(0) = \begin{pmatrix} \frac{1}{3} & \frac{-i}{5} \\ \frac{i}{5} & \frac{2}{3} \end{pmatrix} \quad \Rightarrow \quad \rho_1(0) = \rho_{qm}(0) \otimes \rho_S(0) = \begin{pmatrix} \frac{1}{3} & 0 & \frac{-i}{5} & 0 \\ 0 & 0 & 0 & 0 \\ \frac{i}{5} & 0 & \frac{2}{3} & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

The bases with which these matrices have been written are the typical ones: $\{|+\rangle, |-\rangle\}$, eigenvectors of σ_z, for the two-level system and $\{|n\rangle\}_{n=0}^\infty$ for quantized mode. In addition, it should be noted that here the order indicated above for the tensor product has been reversed, however, it has only been done because it is convenient for the numerical resolution, the physical results will not be altered.

It is also necessary to choose the values of the frequencies and, for this case, the values $\omega_a = 2, \omega_b = 5/2$ and $\omega_c = 6$ have been chosen.

It is important to note that for the initial state of the quantized mode, only the subspace given by $\{|0\rangle, |1\rangle\}$ is being considered. It is necessary to work with subspaces because the base is infinite and in a numerical solution that is immeasurable. However, the fact that the base is infinite is something that must be taken into account when using the Liouville-von Neumann equation, since by making the operators a and $a^\dagger$ act, new terms can appear. For example, when making $a^\dagger$ act on the ket $|1\rangle$, results $a^\dagger|1\rangle = \sqrt{2}|2\rangle$. So, in general, new populations and coherence will appear.

And in fact, that is what happens for the initial condition above, as can be seen in Figure 3.1.

This figure shows the matrix elements in the order that is usually used and with the corresponding notation, so that $\rho_{00} = \langle +, 0|\rho(t)|+, 0\rangle$ and $\rho_{02} = \langle +, 0|\rho(t)|+, 1\rangle$ and so on. But, for simplicity, only non-null matrix elements have been rendered for some instant of time.
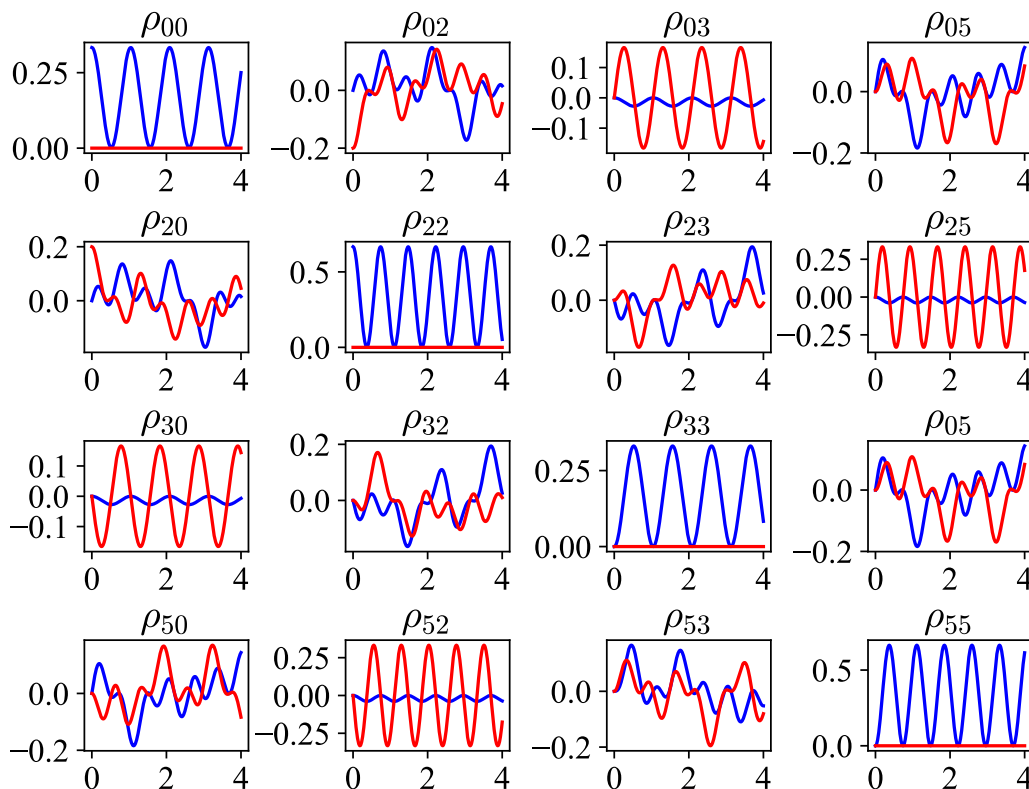
Figure 3.1: Time evolution of matrix elements of the total density matrix with the initial condition $\rho_1(0)$ and taken frequencies $\omega_a = 2, \omega_b = 5/2$ and $\omega_c = 6$ in (3.11). Are shown the ones *different from* 0 at some instant. The imaginary part of each element is shown in red and the real part in blue. The abscissa axis is time in units corresponding to $\hbar = 1$.

In this representation it can be seen that the imaginary part of the diagonal elements is 0 for all t, as it must be true for a density matrix. And the trace remains constant and equal to one. Furthermore, it can be seen that it is hermitic, for example for ρ_{03} and ρ_{30} it can be easily seen that the imaginary parts have the opposite signs. Definitely, the numerical solution appears reliable.

With these results, calculations of total entropy, in each subsystem, entropy production and others can already be made. And in Figures 3.2a and 3.2b all these calculations are shown as a function of time. As for the previous graph, time is in units for which $\hbar = 1$, for the rest of the simulations that are made, this will remain the same. $k_B = 1$ has also been made for these representations and will remain for the rest.

Something remarkable about the Figure 3.2a is that, as might be expected, the total entropy of the system, $S_T(t)$, remains constant. Specifically, for $t = 0$ is obtained $S_T(0) \simeq 0.550686$ and for the last instant that was taken $S_T(4) \simeq 0.550688$. The small difference is the result of having solved the equation of time evolution numerically. That the entropy remains practically constant in time has also been used in the next representations to get an idea of how good the numerical solution is. One more interesting thing in Figure 3.2a is that the total entropy does not coincide with the sum of the entropies of each system separately and, specifically, it is greater than this for every instant of time greater than 0.

Only for $t = 0$ the sum and entropy of the total system coincide. This may sound strange, but it is a general result that will be checked below.
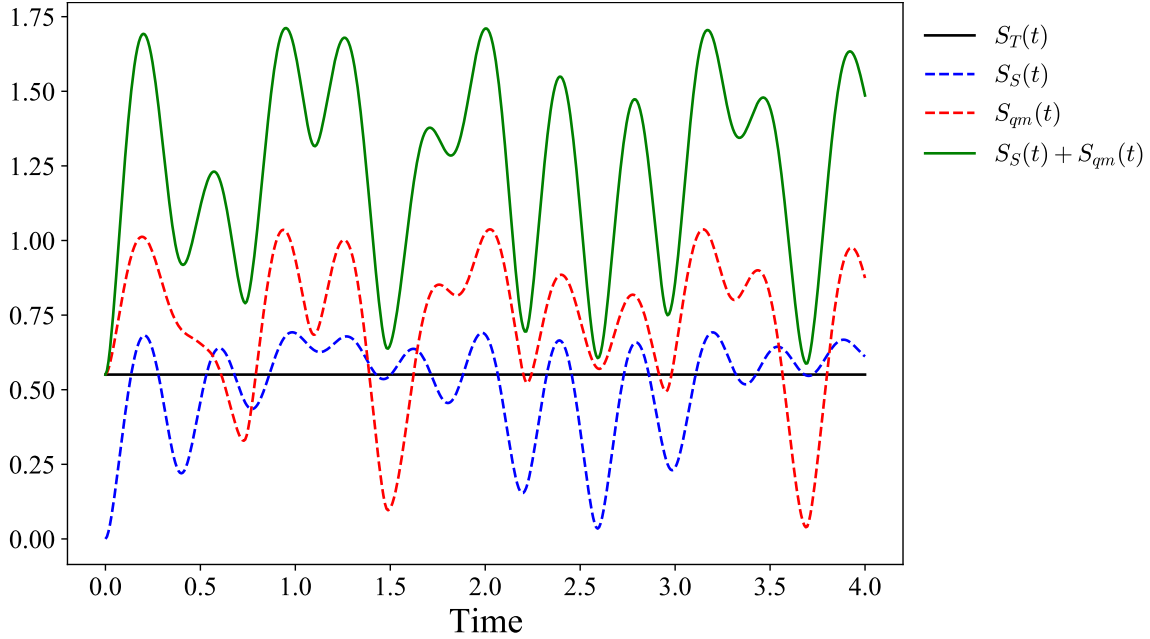
(a) Total entropy, that of each subsystem and the sum of these two.
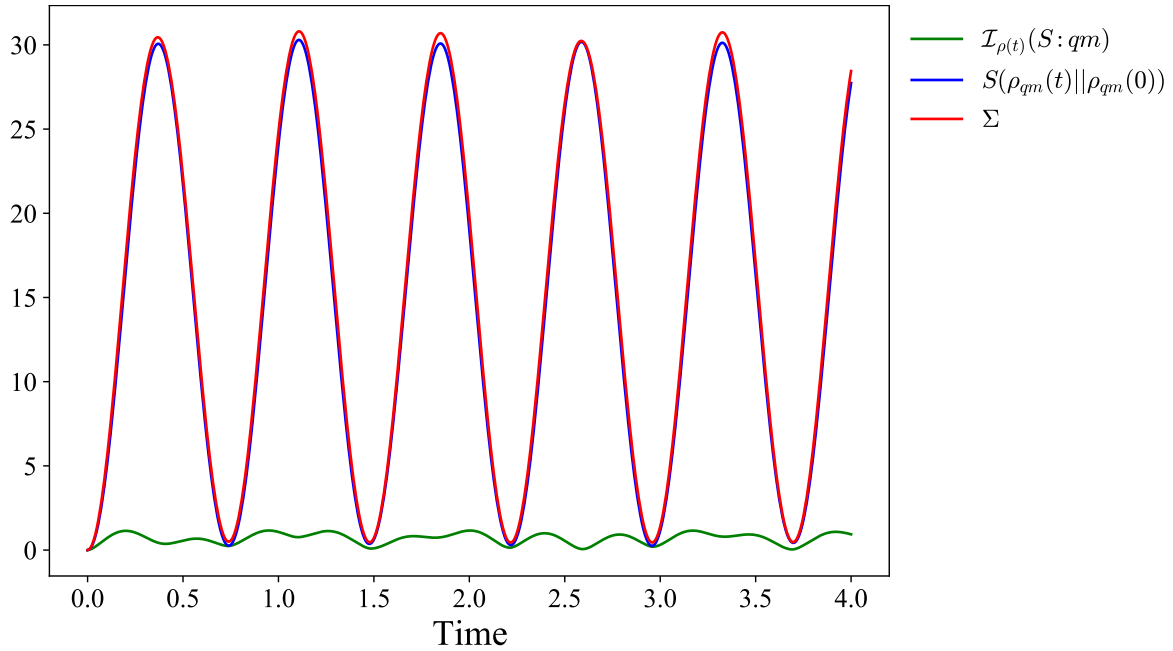
(b) Entropy production and its two contributions, by the relation (3.10).

Figure 3.2: Entropy of the total system, the subsystems and entropy production of the two-level system, S, with its two contributions. Everything calculated with the data shown in 3.1.

First, it was clear that for $t = 0$ the total entropy is the sum of the entropies of each subsystem, since initially the state of the total system was a tensor product. But from that moment on, correlations appear, so **Property 1** is not applicable. This explains why the total entropy does not match the sum for $t \neq 0$.

Second, is defined the "entropy correlation", $S_c(t)$, such that $S_S(t) + S_E(t) + S_c(t) = S_T(t)$, for a total system T composed of a system S and an environment E. In [ELVdB10] it is shown that $S_c(t)$ is an always negative quantity. A demonstration with an alternative and somewhat more detailed procedure will be given here.

To begin with, it is convenient to explicitly write the expressions for entropy:

$$S_S(t) + S_E(t) + S_c(t) = S_T(t) \; \Rightarrow \; S_c(t) = -\operatorname{Tr}\{\rho_T(t)\ln(\rho_T(t))\}+$$
$$+ \operatorname{Tr}\{\rho_S(t)\ln(\rho_S(t))\} + \operatorname{Tr}\{\rho_E(t)\ln(\rho_E(t))\}.$$

Now, according to **Property 2**: $\operatorname{Tr}\{\rho_S(t)\ln(\rho_S(t))\} = \operatorname{Tr}\{\rho_T(t)\ln(\rho_S(t) \otimes \mathbb{1}_E)\}$ and $\operatorname{Tr}\{\rho_E(t)\ln(\rho_E(t))\} = \operatorname{Tr}\{\rho_T(t)\ln(\mathbb{1}_S \otimes \rho_E(t))\}$. Therefore, using the properties of the logarithm:

$$\operatorname{Tr}\{\rho_T(t)\ln(\rho_S(t) \otimes \mathbb{1}_E)\} + \operatorname{Tr}\{\rho_T(t)\ln(\mathbb{1}_S \otimes \rho_E(t))\} = \operatorname{Tr}\{\rho_T(t)\ln(\rho_S(t) \otimes \rho_E(t))\}.$$

With this and comparing this with the definition (3.7), it turns out that it can be written:

$$S_c(t) = -\operatorname{Tr}\{\rho_T(t)\ln(\rho_T(t))\} + \operatorname{Tr}\{\rho_T(t)\ln(\rho_S(t) \otimes \rho_E(t))\} \quad \& \quad (3.7) \; \Rightarrow$$
$$\Rightarrow \; S_c(t) = -S(\rho_T(t)||\rho_S(t) \otimes \rho_E(t)).$$

Therefore, the correlation entropy can be written as the relative entropy and this quantity had the important property of always being greater than or equal to 0, so $S_c(t) \leq 0$, according to the previous result. And this shows that, necessarily, $S_S(t) + S_E(t) \geq S_T(t)$, which is what was necessary to demonstrate.

Finally, something about Figure 3.2b can also be commented. It is quite clear that entropy production has an almost sinusoidal behavior. And the observed minima can be interpreted as instants in which the system S and the quantized mode return to a state similar to the initial one, in which the entropy production was 0. For example, for $t \simeq 2.2$ there is a minimum of Σ and precisely at that moment it can be seen in Figure 3.1 that, in effect, both the populations and the coherence return to a value close to the one they had at $t = 0$. Doing a more exhaustive analysis would not be very useful, since the initial conditions and the chosen frequencies were arbitrary. For example, the initial state of the quantized mode is not a canonical equilibrium state like (3.2), so the relation (3.9), which has a very evident and important classical analogue, would not be applicable. In Section 3.3.2 a more interesting system to analyze Σ can be seen.

The previous system will be analyzed again by introducing different initial conditions and other values of the frequencies, the objective will be to study behaviors of the system that are very interesting.

Specifically, it is considered that $\omega_a = \omega_b$, this results in a resonant behavior. In this case, the quantized mode and the system exchange equal energy quantum, so a totally

periodic behavior of the matrix elements of the system and the quantized mode must be observed.

Moreover, it is interesting to see how many new matrix elements appear based on the initial conditions. Solving the differential equation gives:

$$\rho_S(0) = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \quad \rho_{qm}(0) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad \text{(both in the fund. state)} \rightarrow \begin{array}{c} \text{new matrix elements} \\ \text{do not appear} \end{array}$$

$$\rho_S(0) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad \rho_{qm}(0) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad (1^{st} \text{ excited and fund.}) \rightarrow \begin{array}{c} \text{matrix elements} \\ \text{with } |1\rangle \text{ appear} \end{array}$$

$$\rho_S(0) = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \quad \rho_{qm}(0) = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \quad \text{(fund. and } 1^{st} \text{ excited)} \rightarrow \begin{array}{c} \text{new matrix elements} \\ \text{do not appear} \end{array}$$

$$\rho_S(0) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad \rho_{qm}(0) = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \quad \text{(both in the } 1^{st} \text{ excited state)} \rightarrow \begin{array}{c} \text{matrix elements} \\ \text{with } |2\rangle \text{ appear} \end{array}$$

Taking into account what was mentioned before about the exchange of quanta, with a simple qualitative analysis it is possible to explain this behavior: only when the system is in the excited state do new matrix elements appear, since in that case the system can deliver a quantum to quantized mode and make it go up to another level. Furthermore, since the system can only deliver one energy quanta (it only has one excited level), the quantized mode will only be able to go up one level with respect to the one it had initially, as has been observed.

In any case, whether or not the system is resonant, the two-level will only be able to drive a finite number of levels of the oscillator, but making the system resonant can be more easily understood. Figure 3.3 shows the evolution of the matrix elements with frequencies $\omega_a = \omega_b = 2$ (resonant system) and $\omega_c = 6$ and for the initial condition with:

$$\rho_S(0) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \quad \rho_{qm}(0) = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \Rightarrow \rho_2(0) = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$

Indeed, the periodic behavior of the matrix elements is evident, and the same happens with entropy and entropy production, as can be seen in Figure 3.4. For that case, it turns out that the entropies of the two subsystems are equal and appear superimposed in the figure. It should be noted that it has not been taken into account how the entropy may be "flowing" from one system to another, since it has been considered positive for the two subsystems.

Finally, and to finish the analysis of this model, it is interesting to observe that, since the quantized mode is only excited up to a specific level, the total system is equivalent to the interaction of a two-level system (the S system) and a three-level system (the quantized mode up to the second level excited).

3.3.2 THE RANDOM MATRIX MODEL

This model was proposed in [ELVdB10] in order to illustrate the effectiveness of (3.10) as a proposal for the calculation of entropy production. This model describes the interaction
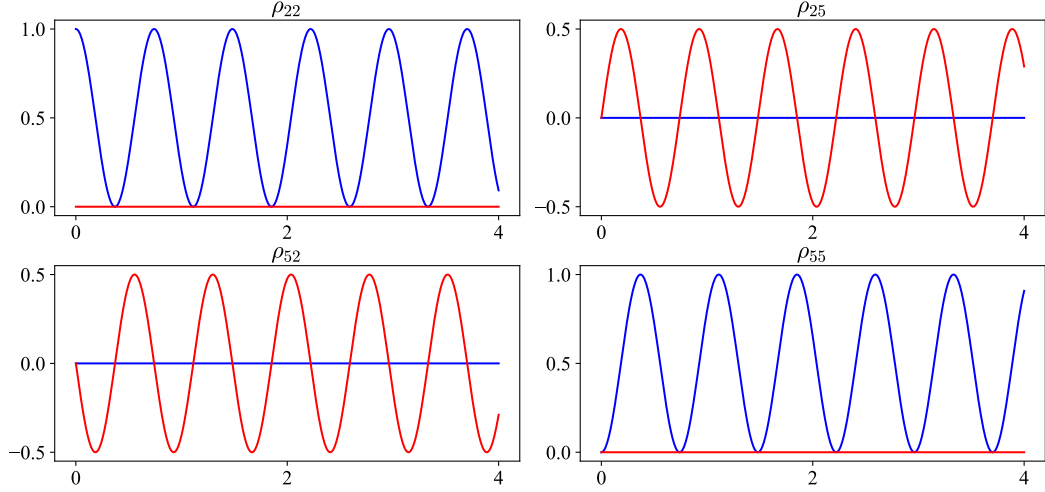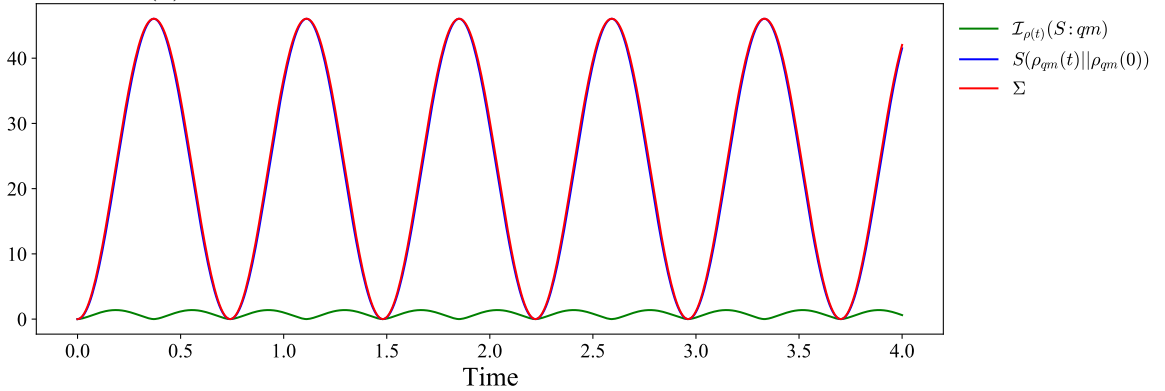
Figure 3.3: Time evolution of matrix elements of the total density matrix with the initial condition $\rho_2(0)$ and taken frequencies $\omega_a = 2, \omega_b = 2$ and $\omega_c = 6$ in (3.11). Are shown the ones *different from* 0 at some instant. The imaginary part of each element is shown in red and the real part in blue.
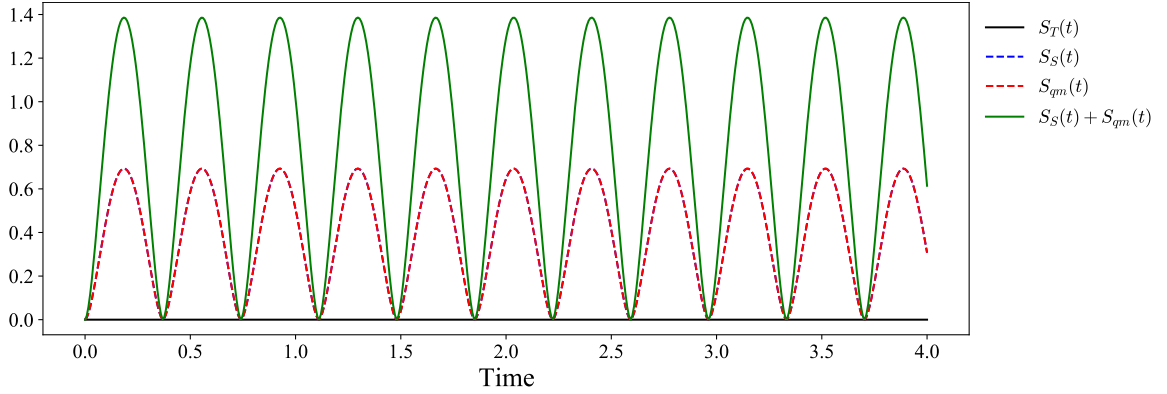
(a) Total entropy, that of each subsystem and the sum of these two.

(b) Entropy production and its two contributions, by the relation (3.10).

Figure 3.4: Entropy of the total system, the subsystems and entropy production of the two-level system, S, with its two contributions. Everything calculated with the data showed in 3.3.

between a 2-level system and a bath of dimension N that is in a canonical equilibrium state, (3.2). Actually, the model is a simple version of the one proposed in [EG03]. But the two cases are characterized by using a Gaussian orthogonal random matrix that describes a environment that has a complex dynamics. These quantum systems are characterized by containing many states interacting with each other and they are common, for example, in quantum chaos.

The hamiltonian with which the total system is described will be:

$$H_G = \frac{\Delta}{2}\sigma_z + H_r + \lambda\sigma_x R, \tag{3.12}$$

where σ_z, again, is the spin operator on the Z axis (analogously for σ_x), H_r is a diagonal matrix with N equally spaced eigenvalues between -0.5 and 0.5. And $R = X/\sqrt{8N}$, with X a Gaussian orthogonal random matrix with probability density proportional to $\exp\{-\operatorname{Tr}\{X^2\}/4\}$.

Information about the formalism on Gaussian orthogonal random matrix can be found in [LNV18]. The procedure to generate the random matrix has been obtained from there and it is quite simple. First, a list is generated of a total of N^2 random numbers obtained from a Gaussian distribution with mean $\mu = 0$ and variance $\sigma^2 = 2$, which comes from set $\exp\{-\operatorname{Tr}\{X^2\}/4\}$. So each number is mapped to each component of a A matrix of dimensions $N \times N$, but this will not result in a hermitic matrix, so finally $X = (A + A^T)/2$ is imposed, with which a physically correct R matrix results.

To reproduce the results of [ELVdB10] the same constants and the same initial conditions have been chosen. Specifically, it has been used for the system and the bath, respectively:

$$\rho_S(0) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \text{ (fundamental state)} \quad \rho_r(0) = \frac{e^{-H_r\beta}}{\operatorname{Tr}\{e^{-H_r\beta}\}} \text{ (canonical equilibrium state).}$$

And with $\Delta = 0.1$, $\lambda = 0.1$ and $\beta = 10$ the result is what is shown in Figure 3.5. In the original article, the system is allowed to evolve for a longer time and for the bath $N = 3, 8, 200$ levels are taken, but to save computational time here it has been allowed to evolve half the time and has reached $N = 100$. However, the results are practically identical. Anyway, the hamiltonian depends on a random matrix, so the original results cannot be exactly reproduced either.

The most curious thing about this result is that it can be perfectly seen how the number of levels of bath affects the production of entropy in the system. For $N = 3$ and $N = 8$ a more or less periodical behavior is obtained for this range of time, but for $N = 100$ the entropy production quickly stabilizes. This was to be expected, it is evident that a smaller bath will not have as much effect on the system.

When a specific system comes into contact with a large bath, as in the previous case, eventually the system will reach a state of thermal equilibrium. It is easy to know what the final state of the system, $\rho_S(f)$, after the contact with the bath has occurred will be [RGWE15]:

$$\text{Weak thermal contact: } \rho_S(f) = \frac{e^{-H_S\beta}}{\operatorname{Tr}\{e^{-H_S\beta}\}}. \tag{3.13a}$$
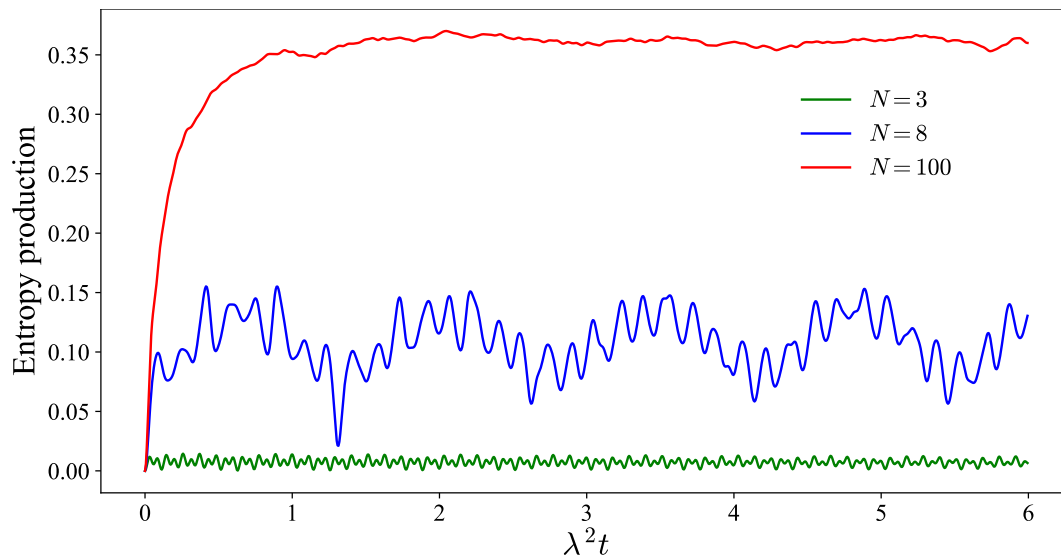
Figure 3.5: Reproduction of the results of [ELVdB10].

$$\text{Beyond weak interaction: } \rho_S(f) = \text{Tr}_B \left\{ \frac{e^{-H\beta}}{\text{Tr}\{e^{-H\beta}\}} \right\}. \tag{3.13b}$$

Where β is the inverse temperature of the bath, H_S the hamiltonian of the system, H the total Hamiltonian and Tr_B denotes the trace over the degrees of freedom of the bath.

Although the authors do not show it in the original article, it can be seen what happened to the state of the two-level system for the case with $N = 100$. This is shown in the next figure, after solving for 100 different random matrices R and carrying out an ensemble average (arithmetic mean of the 100 results) to obtain the final state of the system:
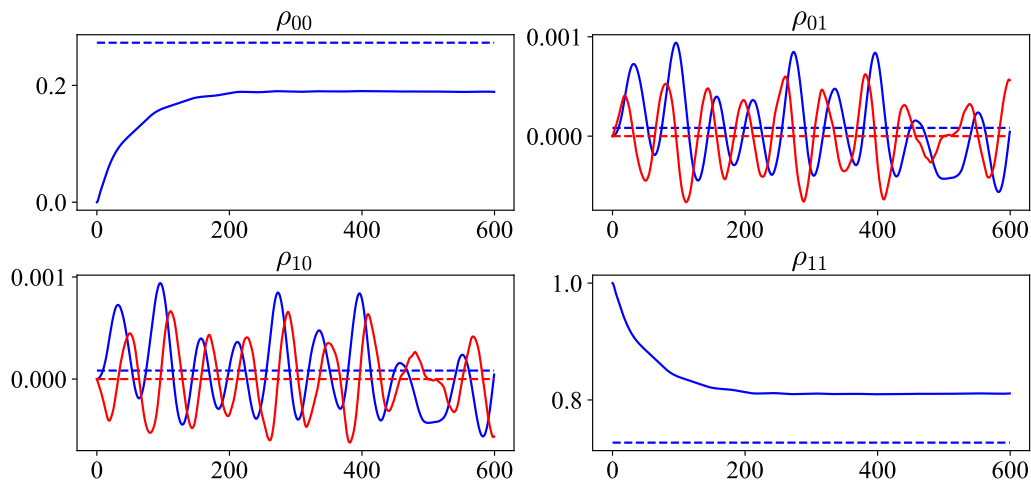

Figure 3.6: Matrix elements of the system after the contact with the bath, with the conditions presented in [ELVdB10] and averaging over 100 contact realizations. Time is shown on the abscissa axis. The imaginary part is shown in red and the real part in blue. In dashed lines can be seen the thermal state to which the system should reach.

To calculate the equilibrium state, the (3.13b) equation was used, although with (3.13a)

the result is something very similar. In any case, there is a considerable discrepancy between this state (with populations $\rho_{00} \simeq 0.2$ and $\rho_{11} \simeq 0.8$) and the thermal state (with populations $\rho_{00} \simeq 0.27$ and $\rho_{11} \simeq 0.73$). And the truth is that the thermal state is not always reached for any type of system and its interaction. According to [RGWE15]:

> For a system to thermalise, we further require:
>
> - Subsystem state independence. if the subsystem is small compared to the bath, the equilibrium state of the subsystem should be independent of its initial state.
>
> - Gibbs form of the equilibrium state.

Indeed, this does not occur for this model, since by choosing a new initial condition for the system, the matrix elements arrive at a different equilibrium state and it is not yet the thermal state. Specifically, this will be verified by choosing a mixed state for the system: $\rho'_S(0) = \begin{pmatrix} \frac{1}{3} & 0 \\ 0 & \frac{2}{3} \end{pmatrix}$. This leads to what is shown in the following figure:
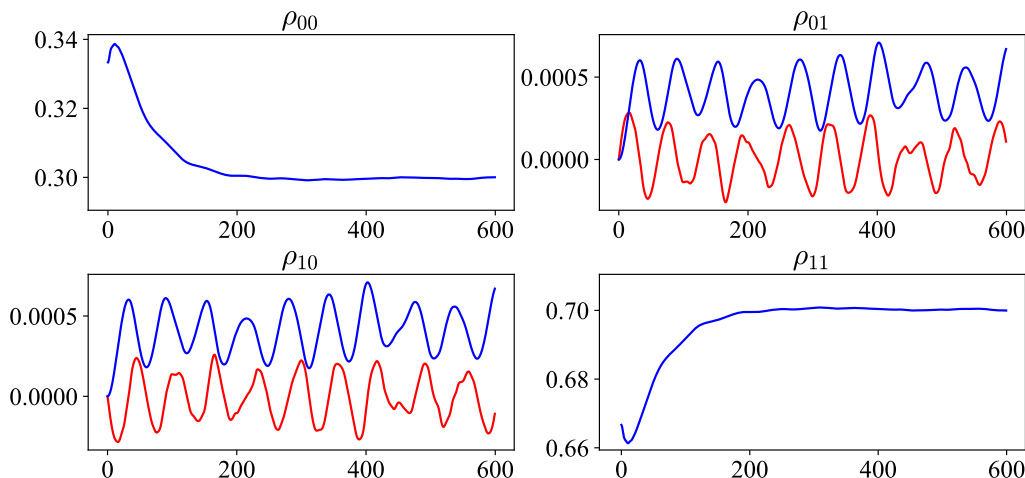

Figure 3.7: Matrix elements of the system after the contact with the bath, with the initial condition $\rho'_S(0)$ and averaging over 100 contact realizations. Time is shown on the abscissa axis. The imaginary part is shown in red and the real part in blue.

In Figure 3.6 it is clear that, for example, the populations stabilize at $\rho_{00} \simeq 0.2$ and $\rho_{11} \simeq 0.8$. But here they stabilize at $\rho_{00} \simeq 0.3$ and $\rho_{11} \simeq 0.7$. Therefore, in effect, *the equilibrium state depends on the initial state*. Obviously, it is possible to know to what state a system that has been in contact with a bath is balanced, but this will not be developed further here. In [RGWE15] the subject is investigated in depth and there are examples of interactions in which something like the above occurs.

Returning to the main topic of this work, it is worth doing an entropy production calculation for the case with $\rho'_S(0)$. In Figure 3.8 the result is shown, together with the curve for entropy production with $N = 100$ from Figure 3.5. It is clear that in the case with the initial condition given by $\rho'_S(0)$ the entropy production stabilizes at a much lower value.
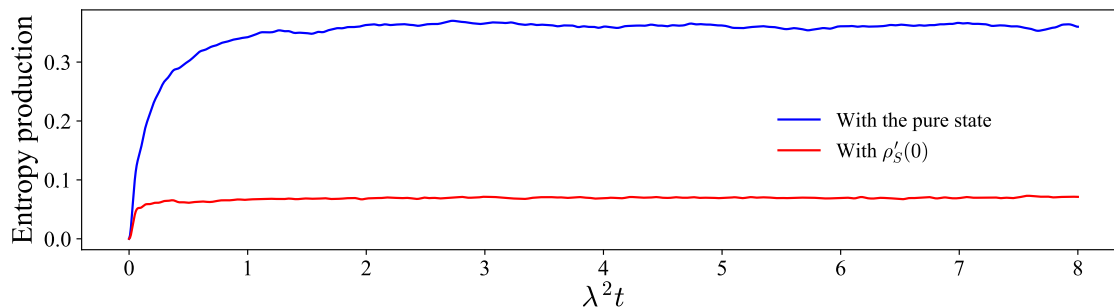
Figure 3.8: Entropy production for $N = 100$ with different initial conditions for the system: the pure and fundamental state and the mixed state $\rho'_S(0)$.

And it is beautiful to see that this agrees with what can be seen in Figures 3.6 and 3.7. In the case of $\rho'_S(0)$ the state in which the system has stabilized is practically the same as the initial state, there is only a difference of hundredths, it goes from 0.33 to 0.3 for ρ_{00} and 0.66 to 0.7 for ρ_{11}, approximately. That is, *the initial and final states are very similar.*

On the other hand, for that case the entropy production is very small and this implies that the uncertainty about the state of the system has not grown too much, so supposing that at time t the state of the system is $\rho_S(t) \simeq \rho'_S(t)$ doesn't go to much of an error. Or what is the same, *the state for an instant of time far from the initial instant is not very different from the initial state.* The two analyzes have reached the same conclusion, which is another sign of the validity of (3.8) as a definition of entropy production in a quantum system.

CHAPTER 4

FLUCTUATION THEOREMS

Resumen

La teoría sobre teoremas de fluctuación apareció hace solo 3 décadas, aproximadamente, y desde su comienzo han sido un tema de investigación muy común. Y no es para menos, ya que el contexto en el que se desarrollan es de lo más general, lo cual los hace útiles para situaciones mucho más allá de la termodinámica básica. En este capítulo solo se dará una breve introducción al tema, empezando por plantear las bases del formalismo y , a continuación, se obtendrán dos teoremas, uno para un caso bien conocido y otro que aparece en un contexto muy concreto, aunque ambos de cierto interés.

4.1 BASIC APPROACH

In the introduction it was mentioned that entropy production appears when studying out-of-equilibrium systems. In all of the above this has not been applied, in fact, there are not many analytical relationships that are valid in those situations. It is in the context where fluctuation theorems that study systems that are arbitrarily out of equilibrium are found [JW04].

The fluctuation theorems can be considered a generalization of the second law of thermodynamics. Normally developments are made with averaged quantities, as is the case with entropy production, but in the formalism of fluctuation theorems this is not the case. The framework will now be more detailed.

A certain system undergoes a process, as is well known, the irreversibility of that process can be quantified by entropy production. That is, after the process: $\Sigma \geq 0$. But this is an averaged value that can fluctuate, so it can be defined: $\varsigma \equiv$ value that can be obtained by observing the entropy production *rate* and that occurs with probability $p(\varsigma)$. Normally, each stochastic realization of the process is called *trajectory*. If the trajectory has elapsed for a time t, the fluctuation theorem states the following [Cro99]:

$$\frac{p(\varsigma)}{p(-\varsigma)} = e^{\varsigma t}. \tag{4.1}$$

And this relationship is valid for systems out of equilibrium.

It is clear that this formula is in perfect agreement with the second law of thermo-dynamics: if the time t is long or the size of the system makes ς very large, the value of $p(-\varsigma)$ gets smaller and smaller, that is, the probability of seeing the entropy decrease ($\varsigma < 0$ implies a decreasing entropy production) vanishes.

The relation (4.1) is not the only way to write a fluctuation theorem. An *anti-trajectory* can be associated with a certain trajectory, which will correspond to carrying out the same process on the system but in reverse. And instead of using the entropy production rate, it is possible to use the entropy production of the trajectory: σ. The corresponding probability distribution can be written as $p(\sigma)$. And it is also possible to associate a distribution to the trajectory reversed: $p^\dagger(\sigma)$. With this, the known Crooks fluctuation theorem takes the form [Cro99, LP20]:

$$\frac{p(\sigma)}{p^\dagger(-\sigma)} = e^\sigma. \tag{4.2}$$

It is useful to work with the σ instead of ς, for example, its average can be identified with the typical entropy production: $\Sigma = \langle \sigma \rangle = \sum \sigma p(\sigma)$.

Crooks' result can be interpreted somewhat more. That relationship implies $\sigma = \ln(p(\sigma)) - \ln\left(p^\dagger(-\sigma)\right)$: each term is like (2.1), that is, the definition given in information theory of the uncertainty associated with an event that occurs with a certain probability (there in units of "bits" and here in "nats"). So the difference is something like a variation of the uncertainty, which is close to the interpretations that had been given previously.

For later studies it will be useful to note that there is one more form of the fluctuation theorem: it is said that the probability distribution $p(\sigma)$ satisfies an *integral* fluctuation theorem if:

$$\langle e^{-\sigma} \rangle = \sum_\sigma p(\sigma)e^{-\sigma} = 1. \tag{4.3}$$

Although this relation is a consequence of (4.2), since it implies that $p(\sigma)e^{-\sigma} = p^\dagger(-\sigma)e^{-\sigma}e^\sigma = p^\dagger(-\sigma) \Rightarrow \langle e^{-\sigma} \rangle = \sum p^\dagger(-\sigma) = 1$.

For all the above, the interest in fluctuation theorems is justified, since the framework for the treatment of entropy production that characterizes them is very general and, as already mentioned in Section 3.2 , finding a general formulation is a problem.

4.2 Fluctuation theorem for (3.8)

With the theory that has been developed, it would be interesting to try to find a fluctuation theorem for the important relation (3.8) that was presented and discussed in the previous chapter. Obviously, this development has already been done. In this work, the procedure presented in [SW21] will be followed.

First, it should be noted that the objective will be to arrive at a relation like (4.1). To do this, it is necessary to know for the case of (3.8) what σ corresponds to and the same for its probability $p(\sigma)$. Furthermore, these values will correspond to a certain initial state and a final state of the system. Thus, the state of the system is denoted at time t and the hamiltonian of the bath as:

$$\rho_S(t) = \sum_\alpha p_\alpha(t) \left|\alpha_t\right\rangle \left\langle\alpha_t\right|_S \quad \& \quad H_B = \sum_k \varepsilon_k \left|\varepsilon_k\right\rangle \left\langle\varepsilon_k\right|_B.$$

And the initial and final states will be given by the measurements in the system and in the bath: $\{|\alpha_0, \varepsilon_k\rangle\} = \{|\alpha_0\rangle \otimes |\varepsilon_k\rangle\}$ and $\{|\alpha_t \varepsilon'_k\rangle\}$.

First, the probability distribution associated to the process is:

$$p[\alpha_t, \varepsilon'_k; \alpha_0, \varepsilon_k] = \langle \alpha_0, \varepsilon_k | \rho_{SB}(0) | \alpha_0, \varepsilon_k \rangle \cdot |\langle \alpha_t, \varepsilon'_k | U_{SB}(t,0) | \alpha_0, \varepsilon_k \rangle|^2 =$$
$$= \frac{e^{-\beta \varepsilon_k}}{\mathcal{Z}} p_\alpha(0) \cdot |\langle \alpha_t, \varepsilon'_k | U_{SB}(t,0) | \alpha_0, \varepsilon_k \rangle|^2,$$

where $\mathcal{Z} = \mathrm{Tr}\{e^{-\beta H_B}\}$ is the partition function. Sometimes that probability is called "path probability" [LP20] and it can be viewed as the product of two probabilities: the one associated to the initial state of the whole system and other that takes into account the process until the final state after the unitary $U_{SB}(t,0)$.

And the expression of the outcome σ corresponding to that probability is not really discussed by the original authors of the article, but with previous results it can be justified. Specifically, with the expression (3.9) for a single bath, where a useful expression for the entropy production can be obtained. Knowing that the expression must have the form $\Sigma = \sum \sigma p(\sigma)$, it is possible to identify the terms for σ:

$$\Sigma = \Delta S_{vN}(\rho_S) - \beta Q \quad \rightarrow \quad \underbrace{\sigma}_{\Sigma} = \underbrace{-[\ln(p_\alpha(t)) - \ln(p_\alpha(0))]}_{\Delta S_{vN}(\rho_S)} - \underbrace{\beta(\varepsilon_k - \varepsilon'_k)}_{\beta Q}.$$

This gives an expression for $e^{-\sigma}$. And, finally, after carrying out the calculations the integral fluctuation theorem for (3.8) is obtained:

$$e^{-\sigma} = \frac{p_\alpha(t)}{p_\alpha(0)} \cdot e^{\beta(\varepsilon_k - \varepsilon'_k)} \quad \Rightarrow \quad \langle e^{-\sigma} \rangle = \sum_{\alpha_t, \varepsilon'_k; \alpha_0, \varepsilon_k} p[\alpha_t, \varepsilon'_k; \alpha_0, \varepsilon_k] \cdot e^{-\sigma} =$$
$$= \sum_{\alpha_t, \varepsilon'_k; \alpha_0, \varepsilon_k} |\langle \alpha_t, \varepsilon'_k | U_{SB}(t,0) | \alpha_0, \varepsilon_k \rangle|^2 \frac{e^{-\beta \varepsilon_k}}{\mathcal{Z}} p_\alpha(0) \frac{p_\alpha(t)}{p_\alpha(0)} \cdot e^{\beta(\varepsilon_k - \varepsilon'_k)} =$$
$$= \sum_{\alpha_t, \varepsilon'_k; \alpha_0, \varepsilon_k} |\langle \alpha_t, \varepsilon'_k | U_{SB}(t,0) | \alpha_0, \varepsilon_k \rangle|^2 \frac{e^{-\beta \varepsilon'_k}}{\mathcal{Z}} p_\alpha(t) = \sum_{\alpha_t, \varepsilon'_k} \frac{e^{-\beta \varepsilon'_k}}{\mathcal{Z}} p_\alpha(t) = 1. \quad \square$$

4.3 Obtaining a fluctuation theorem

In the Section 3.1 it was mentioned that some authors define a generalized form of von Neumann entropy, the operator entropy. This is not the only quantity of this type that is defined in order to give an alternative to the von Neumann entropy, in [SW21] the "observational entropy" is defined and discussed, trying to identify it with the thermodynamic entropy. And, also there, the authors obtain the corresponding fluctuation theorem.

Given the similarity between the definitions that the authors provide for these entropies, a fluctuation theorem for the operator entropy is proposed here. That is, the results of [SW21, Len19] will be used to arrive at a fluctuation theorem, which will be of the particular form of (4.2). And, since there is only interest in obtaining a fluctuation theorem for operator entropy, the advantage of accepting one or the other definition of entropy will not be disputed.

The operator entropy of a system with a density matrix ρ is defined according to a certain operator Q with outcomes q_k and corresponding projectors $|q_k\rangle\langle q_k|$ as:

$$S_Q(\rho) = -\sum_k \text{Tr}\{\rho|q_k\rangle\langle q_k|\} \ln\left(\text{Tr}\{\rho|q_k\rangle\langle q_k|\}\right) = -\sum_k p_k \ln(p_k), \qquad (4.4)$$

where $p_k = \text{Tr}\{\rho|q_k\rangle\langle q_k|\}$ and in the following it will be denoted: $\Pi_k = |q_k\rangle\langle q_k|$. And the corresponding if q_k is degenerate. In this definition it can be clearly seen that the probabilities appear at an intrinsically quantum level as well. Therefore, S_Q reflects an uncertainty arising from the lack of knowledge of the physical world itself, not only the lack of knowledge of the observer, as is the case of von Neumann entropy. The observational entropy is similar, it has two terms, one is equal to $S_Q(\rho)$ and the other is $\sum_k p_k \ln(V_k)$, where $V_k = \text{Tr}\{\Pi_k\} \equiv$ dimension of Π_k.

As in the previous section, it is necessary to have a probability distribution (two distributions in this case, because the final result has the form (4.2)) and the corresponding expression of the entropy production in a trajectory. And, since ρ corresponds to a system that is considered isolated, it is easy to define:

$$\Delta s_Q = s_Q(t) - s_Q(0) = -(\ln(p_{k_t}) - \ln(p_{k_0})) = \ln\left(\frac{p_{k_0}}{p_{k_t}}\right).$$

Regarding the probability distribution, it is more complicated. First, it is necessary to define the probability of observing the outcomes q_{k_0} and q_{k_t} (at 0 and t respectively) in the "forward process". And it turns out that that probability is: $p_{0t} = \text{Tr}\{\Pi_{k_t}U(t)\Pi_{k_0}\rho(0)\Pi_{k_0}U^\dagger(t)\}$, where $U(t)$ is the unitary that has brought the system to its state in t. Now it is possible to find the probability of obtaining a Δs value from the variation of the entropy operator by the expression:

$$p(\Delta s) = \sum_{k_0,k_t} p_{0t} \cdot \delta\left(\Delta s - \Delta s_Q\right).$$

The Dirac delta function is introduced to account for any possible value of the variation of s_Q equal to Δs, taking into account that this can be for any pair of outcomes of k_0 and k_t. To continue with the development it is necessary to make a first assumption, which is quite restrictive, it will be assumed that at the initial instant: $\rho(0) = \sum_{k_0} p_{k_0}\Pi_{k_0}/V_{k_0}$. So:

$$p(\Delta s) = \sum_{k_t,k_0} \text{Tr}\{\Pi_{k_t}U(t)\Pi_{k_0}\rho(0)\Pi_{k_0}U^\dagger(t)\} \cdot \delta\left(\Delta s - \Delta s_Q\right) =$$

$$= \sum_{k_t,k_0} \text{Tr}\{\Pi_{k_t}U(t)\Pi_{k_0}U^\dagger(t)\}\frac{p_{k_0}}{V_{k_0}} \cdot \delta\left(\Delta s - \Delta s_Q\right) =$$

$$= \sum_{k_t,k_0} \text{Tr}\{\Pi_{k_0}U^\dagger(t)\Pi_{k_t}U(t)\}\frac{p_{k_t}}{V_{k_0}}\exp\left[\underbrace{\ln\left(\frac{p_{k_0}}{p_{k_1}}\right)}_{\Delta s_Q}\right] \cdot \delta\left(\Delta s - \Delta s_Q\right) =$$

$$= e^{\Delta s}\sum_{k_t,k_0} \text{Tr}\{\Pi_{k_t}U(t)\Pi_{k_0}U^\dagger(t)\}\frac{p_{k_t}}{V_{k_0}} \cdot \delta\left(\Delta s - \Delta s_Q\right).$$

For the second equality it has been used that $\Pi_{k_0}\rho(0)\Pi_{k_0} = \Pi_{k_0}p_{k_0}/V_{k_0}$, for the third $p_{k_0}/V_{k_0} = p_{k_t}$ and $\mathrm{Tr}\{AB\} = \mathrm{Tr}\{BA\}$. And for the last equality the delta function was used to put $e^{\Delta s_Q}$ out of the sum.

Now the second assumption will be made, which will be $V_{k_0} = V_{k_t}$ (this is not $k_0 = k_t$, it is only the equality of the dimensions). The $\mathrm{Tr}\{\Theta A\Theta^{-1}\} = \mathrm{Tr}\{A\}^*$ property will also be used, where Θ is the time-reversal operator, which describes the process that the system undergoes, but in the opposite "direction". And the operators in this case should be denoted as $A^\Theta = \Theta A\Theta$. With that, and putting the factor p_{k_t}/V_{k_t} inside the trace:

$$
p(\Delta s) = e^{\Delta s} \sum_{k_t,k_0} \mathrm{Tr}\left\{ \Pi_{k_0}^\Theta U_\Theta(t)\Pi_{k_t}^\Theta \overbrace{\sum_{k_t'} \frac{p_{k_t'}\Pi_{k_t'}^\Theta}{V_{k_t'}} \Pi_{k_t}^\Theta U_\Theta^\dagger(t)}^{p_\Theta(-\Delta s)} \right\} \delta\left(\Delta s - \Delta s_Q\right) \quad \Rightarrow
$$

$$
\Rightarrow \quad \boxed{\frac{p(\Delta s)}{p_\Theta(-\Delta s)} = e^{\Delta s}} \tag{4.5}
$$

Finally, it should be pointed out what $p_\Theta(-\Delta s)$ is, it is the probability of obtaining an operator entropy production of Δs in the process given by: a initial state in $\sum_{k_t} p_{k_t}\Pi_{k_t}^\Theta/V_{kt}$, the measure of Q_t^Θ, the evolution in time reversed direction and the measure of Q_0^Θ. The subscript in the operators indicates that they may not be the same in 0 and in t.

It should be noted that a more general fluctuation theorem than this can possibly be obtained, since it has been developed by setting somewhat severe constraints. However, it is shown that the definition of entropy (4.4) also admits a fluctuation theorem, as would be expected from a consistent definition of entropy. With all, the importance of fluctuation theorems is proven, although the mathematical tools are somewhat more complex than in other formalisms, they provide powerful tools for studies of systems in many situations.

CHAPTER 5

CONCLUSIONS

Since the beginning, it had been clear that entropy production is a quantity of capital importance when one wants to study any process that a system undergoes. With this in mind, it is clear that a correct and detailed understanding of what entropy and entropy production are is necessary.

Although the Chapter 2 only gives a not very broad basis of what it is necessary to know about information theory, it has turned out that the knowledge of that discipline that is exposed there, together with the examples and reasoning that arise, have been enough to give an interpretation (both to the results of obtaining expressions and also numerical solutions) of the entropy that appear in the rest of the chapters.

One of the fundamental parts of this work has been the work until reaching the relation (3.8). But the truth is that this is not such a complex relationship and obtaining it becomes trivial if basic properties are available on traces, density matrices, tensor products... This simplicity may be a sign that the starting hypotheses were too restrictive. For example, to arrive at a formula for entropy production it would have been possible at first to suppose that irreversibility arises from the information that is lost on the state of baths when tracing on their degrees of freedom. But this leaves a term out of the game, mutual information, which does appear in (3.8). So, could a term that contributed to entropy production have been lost?

The truth is that the reasoning followed by the original authors seems solid within their hypotheses. Not only that, the numerical calculation of solutions for specific systems gave the expected results. The Jaynes–Cummings model allowed to show that the behavior of the entropy is the one that could be expected within the proposed situation to arrive at (3.8). However, it is perhaps a slightly more complex model than necessary for that purpose, since computationally it was not very easy to include in the program the fact that the dimension of the Hilbert space of the harmonic oscillator is infinite.

Another interesting model was that of the Section 3.3.2, where it was possible to verify that the numerical solutions that had been made were correct, since the results of the authors who originally proposed the model could be reproduced. Specifically, the study of the two-level system alone led to very interesting conclusions. In particular, the one whereby the entropy production was, as might be expected, lower when the state of the system in t did not change much with respect to the initial state.

However, a problem arose: the final state of the system could not be determined after

the contact occurred. Although it was possible to find how to solve this in the literature, it was preferred not to investigate so much in such a specific detail. But it would be interesting to see if it is possible to find, by means of the appropriate formalism, an initial state for which the entropy production is almost zero, so that during some time the dynamics would be close to being reversible even if the bath was very large.

Finally, although the subject was not investigated too much, it was possible to reveal the framework in which the fluctuation theorems appear. It was even possible to obtain two theorems, one well known (for the relation 3.8) and the other quite specific that, in principle, could be useful in a very concrete situation. In general, fluctuation theorems appear with relatively complex mathematical tools, which makes their manipulation difficult. However, considering the problem of giving a general formulation for entropy production, it is worth investigating further. And, indeed, it seems that this is one of the most promising directions for important future results.

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