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Contribuições da coerência para a produção de entropia em processos quânticos

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Coherence contributions to the entropy production in quantum processes

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Fim de tarde.
No céu plúmbeo
A Lua baça
Paira
Muito cosmograficamente
Satélite.

Desmetaforizada,
Desmitificada,
Despojada do velho segredo de melancolia,
Não é agora o golfão de cismas,
O astro dos loucos e dos enamorados,
Mas tão somente
Satélite.

Ah Lua deste fim de tarde,
Demissionária de atribuições românticas,
Sem show para as disponibilidades sentimentais!

Fatigado de mais-valia,
Gosto de ti assim:
Coisa em si,
– Satélite.

— Manuel Bandeira, *Satélite*

Resumo

A termodinâmica de processos quânticos é um campo de estudo recente e que tem crescido nos últimos anos. Anteriormente pensada como um fenômeno emergente para sistemas macroscópicos, a termodinâmica pôde ser aplicada a sistemas quânticos considerando quantidades como calor e trabalho como estocásticas. A particularidade desses sistemas é que, além de estudar recursos energéticos, devemos levar em consideração também recursos informacionais quânticos como emaranhamento e coerência.

Nesse cenário, a entropia se torna uma quantidade importante, pois além de estar relacionada à irreversibilidade de um processo, ela também pode ser usada como medida da quantidade de informação do sistema a que temos acesso. A entropia, diferentemente da energia, não é uma quantidade conservada; isso é, em um sistema fechado, não há somente fluxo de entropia entre partes deste como há também, em geral, produção de entropia. De acordo com o princípio de Landauer [1], é a entropia produzida que tem como contrapartida a perda de informação. Estudar, então, a produção de entropia torna-se importante para áreas como computação quântica, onde se deseja ter controle sobre ganhos e perdas de informação.

Em processos quânticos, a produção se dá tanto devido a mudanças na energia do sistema quanto a flutuações na coerência [2, 3], um recurso puramente quântico. Neste projeto, propomos estudar a estatística da produção de entropia devido à coerência. Para isso, investigaremos duas divisões diferentes da produção de entropia: a proposta em [2, 3] e a outra apresentada em [4, 5]. Por simplicidade, analisaremos um processo quântico unitário, usando o esquema de medição em dois pontos [*two-point measurement* (TPM) *scheme*] [6]. Aplicaremos ambos os formalismos para dois sistemas quânticos específicos: um modelo de macrospin e o modelo Lipkin-Meshkov-Glick (LMG) [7–9]. Analisaremos, nesses casos, como a distribuição da coerência depende de parâmetros como dimensão do sistema, temperatura, tempo de evolução, etc.

Palavras-chave: Termodinâmica quântica; Produção de entropia; Informação quântica; Coerência; Processos de não-equilíbrio.

Abstract

The thermodynamics of quantum processes is a recent field of study and it has been growing in recent years. Previously thought of as an emergent phenomenon for macroscopic systems, thermodynamics started being applied to quantum systems considering quantities such as heat and work as stochastics. The peculiarity of these systems is that, in addition to studying energetic resources, we must also take into account quantum informational resources such as entanglement and coherence.

In this scenario, entropy becomes an important quantity, because in addition to being related to the irreversibility of a process, it can also be used as a measure of the amount of information in the system to which we have access. Entropy, unlike energy, is not a conserved quantity; that is, in a closed system, there is not only an entropy flow between it's parts, but also, in general, entropy production. According to the principle of Landauer [1], it is the entropy produced that causes the loss of information. Studying, then, the production of entropy becomes important for areas such as quantum computing, where you want to have control over information gains and losses.

In quantum processes, entropy is produced due both to changes in the energy of the system and to fluctuations in coherence [2, 3], a purely quantum resource. In this project, we propose to study the statistics of entropy production due to coherence. For this, we will investigate two different splittings of the entropy production: the one proposed in [2, 3] and a most recent one proposed in [4, 5]. For simplicity, we will analyse a unitary quantum process, using the two-point measurement (TPM) scheme [6]. We will apply both formalisms for two specific quantum systems: a macrospin model and the Lipkin-Meshkov-Glick (LMG) model [7–9]. We will analyse, in these cases, how the distribution of coherence depends on parameters such as system dimension, temperature, evolution in time, etc.

Keywords: Quantum thermodynamics; Entropy production; Quantum information; Coherence; Non-equilibrium processes.

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Chapter 1

Introduction

Heat and work have always been important forms of energy to humankind. Heat has been broadly used as a resource, since the discovery of fire, going through the first industrial revolution, when heat engines started to be used as a source of power to operate machines, until nowadays when we use it in the everyday life. Work, on the other hand, is present whenever a body exerts a force on another; it allows us to walk, cars to move, refrigerators to cool and electricity to be generated by wind or hydroelectric power stations. It has always been of great importance to comprehend and be able to manipulate heat and work [11, 12], and due to that need thermodynamics is still an active field of research.

Thermodynamics was previously thought of as the study of systems through their macroscopic properties such as pressure, volume and temperature. Nonetheless, it started being applied to microscopic systems when James Clerk Maxwell and Ludwig Boltzmann proposed that those characteristics emerged as an average collective behavior of multiple minuscule particles. That knowledge enabled the development of statistical mechanics, which besides dealing with averages, also modeled the probabilistic behavior of individual particles.

However, upon stepping into the microscopic world, quantum features must be taken into account. Then came the field of *quantum thermodynamics*, that besides proposing new definitions of heat, work and temperature for quantum systems, presented how strictly quantum aspects such as entanglement and coherence could also be used as resources [13–15]. For example, it has been shown that coherences can be employed to enhance work extraction [16–22] and heat engine efficiency [23–26]. At the stochastic level, they can contribute to work and heat fluctuations [27–31] and generate local violations of the second law [32–35].

Like heat and work, entropy has also been broadly studied in the context of quantum ther-

modynamics, as well as quantum information and computation. The concept was one of the bridges between classical thermodynamics and the microscopic world, as Boltzmann proposed that entropy quantifies the possible number of microstates of a system. It also entered the quantum realm through information theory; von Neumman extended the notion of Shannon entropy to quantify information in quantum systems [36].

Besides entropy itself, entropy production is also notably relevant to quantum information and quantum thermodynamics. When talking about information, it is a key concept as it is directly linked to the irreversibility of processes and information erasure [1]. With experimental advances allowing for the construction of quantum superpositions, the storage and transmission of information was revolutionized, and so it became necessary to comprehend the role of entropy production in quantum processes and how quantum features may influence the increase in entropy.

In the context of thermodynamics, entropy production is also associated to irreversibility. Consider, for example, a classical system with two subsystems at temperatures T_A and T_B, $T_A > T_B$. Heat will spontaneously flow from subsystem A to B until they thermalize, but it will not flow from B to A. In this irreversible process, entropy is produced, even though the process is done in a *quasi-static* manner (i.e., the system goes through a succession of equilibrium states) [11]. Other than that, processes which are not quasi-static always increase entropy. For instance, consider the following *work protocol*: a system is in thermal equilibrium with a bath, and an external parameter is changed such that it is taken to a non-equilibrium state. We can think of a piston rapidly compressing a gas or a rubber band being abruptly stretched [37]. These kinds of processes are also irreversible and therefore lead to entropy production.

Notwithstanding, when considering the thermodynamics of quantum systems, entropy production stems not only from changes in energy, which can be considered a classical feature, but also from coherences [2, 3], a purely quantum resource that can be associated to a basis rotation (Fig. 1.1). The objective of this work is to determine how coherence contributes stochastically to the total entropy production. This is not a straightforward task, as there is no unique way to separate the two different contributions.

In the present work, we will deal with entropy production due to work protocols as defined above. We will present two different splittings for the entropy production proposed in the literature. The first one, proposed in References [2, 3], considers that the entropy production due to coherences comes from the entropic distance between the final state of the system and its

Figure 1.1: Entropy production in a quantum system can be due to changes in the energy levels or due to basis rotation (that produces coherences) [5].

diagonal version. The second splitting, recently proposed in References [4, 5], acknowledges that entropy production should be split according to its dependence on the diagonal or coherent parts of the drive Hamiltonian.

The dissertation is divided as follows. In Chapter 2, we introduce some fundamental contents of Quantum Mechanics that are needed to understand the work developed. We assume that the concepts of Hilbert space, states (including Dirac's representation as *bras* and *kets* [38]), operators, time evolution (Schrödinger equation) and spin theory are known. In Chapter 3, we gather some information about entropy production in the context of classical and quantum thermodynamics and information theory.

Chapter 4 is about the models used for numerical applications of this work: a macrospin system and the Lipkin-Meshkov-Glick (LMG) model [7–9]. We expose how the total entropy production behaves in each of them. Afterwards, in Chapters 5 and 6, we enter the main subject of this project. We present the two different splittings to the entropy production [2–5], and analyse how each of them behaves stochastically and as a function of the system's parameters. For concreteness purposes, we apply the result to the models previously presented. Finally, in Chapter 7, we exhibit some final considerations and propose possible future works our project may lead to.

Throughout the dissertation, we will employ natural units: $k_B = \hbar = 1$.

Chapter 2

Quantum mechanics

The theory of Quantum Mechanics is built mainly around states and operators; a system at any time is represented by a state, and most changes in the system (evolution, interaction, measurement) are represented by operators. To operate with the theory, we generally use linear algebra: states and operators correspond to vectors and matrices in a complex vector space (the Hilbert space), the size of which depends on the dimension of the system. Since the introduction of Dirac's notation [38], we use *kets* and *bras* to write vectors and dual vectors, respectively. Nonetheless, this representation has a shortcoming: not all states can be expressed in this form. As we will see, some states need to be represented as matrices.

2.1 Density matrix

Any system state that can be represented by a ket $|\psi\rangle$ can also be represented by a matrix, by taking the outer product of $|\psi\rangle$ with its dual vector $\langle\psi|$,

$$\rho = |\psi\rangle\langle\psi|. \tag{2.1}$$

The resultant matrix is called a *density matrix* or *density operator*. For states such as the above, that can be represented by kets, the density matrix contains no more information than the vector itself. For instance, in the case of a qubit (2-level system), if $|\psi\rangle = a|0\rangle + b|1\rangle$, with $|0\rangle = (1,0)^\intercal$, $|1\rangle = (0,1)^\intercal$ and $a^2 + b^2 = 1$, the corresponding density matrix will be

$$\rho = (a|0\rangle + b|1\rangle)(a^*\langle0| + b^*\langle1|) = |a|^2 |0\rangle\langle0| + |b|^2 |1\rangle\langle1| + ab^* |0\rangle\langle1| + a^*b |1\rangle\langle0|,$$

that is,

$$\rho = \begin{pmatrix} |a|^2 & ab^* \\ a^*b & |b|^2 \end{pmatrix}. \tag{2.2}$$

States that can be written as kets are called *pure states*. This is related to the definition of *purity* [39],

$$\mathcal{P} := \mathrm{tr}(\rho^2), \tag{2.3}$$

where $\mathrm{tr}(\sigma) = \sum_i \sigma_{ii}$ is the sum of the diagonal elements of a matrix σ. The purity is always smaller or equal to 1 ($\mathcal{P} \leq 1$), the equality being valid only when ρ is a pure state. However, the density operator is most useful in cases where a system's state cannot be written in the form of a vector, that is, when the system is in a *mixed state* (in opposition to a pure state). Consider a system that, with some probability p, is in the state $|\psi_1\rangle$ and with probability $(1 - p)$ is in the state $|\psi_2\rangle$ [40]. Notice that, in the last example, the system was in a quantum superposition, which is not the case here. The uncertainty associated with the system's state is of purely classical nature [39]. Its density matrix will be

$$\rho = p\,|\psi_1\rangle\langle\psi_1| + (1 - p)\,|\psi_2\rangle\langle\psi_2|.$$

It is not possible to write this matrix as the outer product of only one vector with its dual.

A density operator's general form is

$$\rho = \sum_i p_i\,|\psi_i\rangle\langle\psi_i|, \tag{2.4}$$

where $\{|\psi_i\rangle\}$ is the eigenbasis of the system and p_i are the eigenvalues, or else probabilities, associated with each state i. This kind of operator obeys two properties that can be easily derived by taking into account the already known properties of vector states: (1) it has trace equal to one, and (2) is positive semi-definite [36, 40]. In this framework, the average of an operator is defined as [40]

$$\langle A \rangle := \mathrm{tr}(A\rho) = \sum_i p_i\,\langle\psi_i|A|\psi_i\rangle. \tag{2.5}$$

When talking about time evolution of density matrices, we need to generalize Schrödinger's equation. First, recall that if a system evolves from a time t_0 to a time t according to its (time-

independent) Hamiltonian H, the final state will be given by

$$|\psi(t)\rangle = U(t, t_0) |\psi(t_0)\rangle, \tag{2.6}$$

where $U = \exp\{-iH(t - t_0)\}$ and $|\psi(t_0)\rangle$ is the initial state. This is valid for any pure state. For a general state [Eq. (2.4)], we consider that each of its eigenstates $|\psi_i(t_0)\rangle$ evolves according to Eq. (2.6). So the whole state evolves as

$$\rho(t) = \sum_i p_i \, U(t, t_0) |\psi_i(t_0)\rangle\langle\psi_i(t_0)| \, U^\dagger(t, t_0) = U(t, t_0) \, \rho(t_0) \, U^\dagger(t, t_0). \tag{2.7}$$

Equation (2.7) above shows that a unitary evolution does not change the eigenvalues of a system, only its eigenvectors; it can thus be interpreted as a basis rotation. If we differentiate both sides with respect to t and make some adjustments, we obtain the so called *von Neumann's equation* [39],

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = -i[H, \rho]. \tag{2.8}$$

Unitary transformations are only some of many operations that may be done to a quantum system's state. Any operation can be written as a *map*, such as [36]

$$\rho' = \mathcal{E}(\rho), \tag{2.9}$$

that is, the map $\mathcal{E}$ takes ρ into ρ'. In the unitary case, $\mathcal{E}(\rho) = U\rho\, U^\dagger$. But, for some map to represent a possible physical transformation, it is necessary that it takes valid density matrices to valid density matrices, i.e., the state $\mathcal{E}(\rho)$, just like ρ, has to obey the properties previously enunciated so that it represents a physical state. The maps that fulfill this conditions are called *Completely Positive Trace Preserving* (CPTP) maps. They may be represented by *Kraus operators* as [39, 41]

$$\mathcal{E}(\rho) = \sum_k M_k \rho M_k^\dagger, \tag{2.10}$$

with $\sum_k M_k M_k^\dagger = 1$. It is easy to notice that unitaries are CPTP maps; let all $M_k = 0$ except for one $M_i = U$, then $\mathcal{E}(\rho) = U\rho\, U^\dagger$ is a valid Kraus representation of a map that preserves the trace and positivity of density matrices.

At last, let us develop some intuition about the density matrices' elements. The most general form of a density operator on a 2-dimensional Hilbert space [39] which obeys the properties

enlisted is

$$\rho = \begin{pmatrix} p & q \\ q^* & 1-p \end{pmatrix}. \tag{2.11}$$

It is noticeable that its diagonal elements are associated with the probabilities of finding the qubit in the computational basis, as we said earlier. This remains true for any dimension. The off-diagonal elements have no classical interpretation; those are called *quantum coherences*. We shall explain them more in detail in Section 2.2.

2.1.1 Composite systems and partial trace

Density matrices are also used to represent composite system's states. Consider, for example, the case of two qubits. If both are in pure and uncorrelated states, their composite state is a linear combinations of $|0,0\rangle$, $|0,1\rangle$, $|1,0\rangle$ and $|1,1\rangle$. However, for mixed or correlated states, Dirac's notation is not enough.

If the systems are mixed but independent, their states can be written using the *tensor* or *Kronecker product* [39]. A state $|i,j\rangle$ is given by

$$|i,j\rangle = |i\rangle \otimes |j\rangle. \tag{2.12}$$

These are called *product* or *separable states*. The tensor product is used to show that each state belongs to its own Hilbert space; it is possible to operate with one qubit while leaving the other undisturbed. Nonetheless, the same notation is valid for density matrices. For example, if the qubits are in states ρ_A and ρ_B, their global state is $\rho_{AB} = \rho_A \otimes \rho_B$. In matrix notation, ρ_{AB} is given by

$$\rho_{AB} = \begin{pmatrix} \rho_{11}^A \, \rho_B & \rho_{12}^A \, \rho_B \\ \rho_{21}^A \, \rho_B & \rho_{22}^A \, \rho_B \end{pmatrix}, \tag{2.13}$$

where ρ_{ij}^A are the matrix elements of ρ_A. Note that each element multiplies the whole matrix ρ_B, so the result is a 4×4 matrix.

Notwithstanding, the most general possible state of a composite system cannot be expressed using the tensor product, as the subsystems may be correlated. They are represented by matrices that belong to a Hilbert space of dimension $d_1 \times d_2 \times ... \times d_N$, where d_i is the dimension of the Hilbert space of system i.

Although it is not possible to write states of correlated systems with tensor products, it

is possible to obtain some information about the individual subsystems by using an operation called *partial trace*. Looking at the product state ρ_{AB} again, we define $\{|a\rangle\}$ as the eigenbasis of ρ_A and $\{|b\rangle\}$ as the eigenbasis of ρ_B; the composite system's eigenbasis is, then, $\{|a,b\rangle\}$. The trace of ρ_{AB} is given by [39]

$$
\begin{aligned}
\text{tr}(\rho_{AB}) &= \sum_{a,b} \langle a,b|\rho_{AB}|a,b\rangle \\
&= \sum_{a,b} ((\langle a| \otimes \langle b|)(\rho_A \otimes \rho_B)(|a\rangle \otimes |b\rangle)) \\
&= \sum_a \langle a|\rho_A|a\rangle \sum_b \langle b|\rho_B|b\rangle \\
&= \text{tr}(\rho_A)\,\text{tr}(\rho_B).
\end{aligned}
\tag{2.14}
$$

The final result of the trace over both Hilbert spaces is a number. The partial trace is defined such that we trace over only one of the Hilbert spaces and the final result is a matrix with support on the space we did not trace. In the case of ρ_{AB}, the partial traces over A and B yield, respectively,

$$
\text{tr}_A(\rho_{AB}) = \text{tr}(\rho_A)\rho_B, \qquad \text{tr}_B(\rho_{AB}) = \rho_A\,\text{tr}(\rho_B).
\tag{2.15}
$$

In the case of separable states, we notice that, as the trace of any density matrix is 1, the trace over one subsystem gives as a result the density matrix of the other subsystem. That is,

$$
\rho_A = \text{tr}_B(\rho_{AB}), \qquad \rho_B = \text{tr}_A(\rho_{AB}).
\tag{2.16}
$$

The result of Eq. (2.16) is general: it is valid even if ρ_{AB} is not a separable state. The matrices ρ_A and ρ_B are called the *reduced density matrices* of the composite system [39]. The same logic can be applied for multipartite systems of any dimension. For example, given a tripartite state ρ_{ABC}, we can trace over one or more subspaces, such as $\rho_A = \text{tr}_{B,C}(\rho_{ABC})$ or $\rho_{AB} = \text{tr}_C(\rho_{ABC})$.

If the subsystems are correlated, i.e., their global state can't be expressed as a product state, the operation of taking the partial trace does not preserve information about the composite system in its entirety. When the state is separable, the global density matrix can be reconstructed from the reduced ones: it suffices to take their tensor product. But it is not the case for an unseparable state; the global density matrix cannot be recovered from the reduced ones, because we have eliminated the correlations by taking the partial trace.

2.2 Quantum coherence

The study of quantum coherences initially began in the field of optics [42, 43], through the study of "phase space distributions and multipoint correlation functions" [44]. However, quantum coherences proved to be very useful in other fields as well. Just like heat and work are viewed as energetic resources in classical physics, which can be consumed to perform tasks, quantum correlations such as coherence and entanglement can be thought of as quantum resources with the emergence of quantum information theory [44, 45]. That motivates the definition of coherence measures, that is, a way of quantifying coherence such that it is possible to associate an amount of coherence to each state and compare them [44].

But before we start talking about coherence quantifiers, we shall make an important remark: coherence is intrinsically dependent on the basis chosen to describe the system. We said that, in Eq. (2.11), the off-diagonal elements are the coherences. But density matrices are diagonalizable, and written in its own eigenbasis a density operator has no off-diagonal elements. So, how can we tell if a system has coherences or not?

This problem is solved by considering that there could be a *preferred basis* by the system. The basis is usually determined by the interaction of the system with an environment, and takes into account what is being measured [46, 47]. There is no need for an actual measurement to be performed; by interacting with the system, the environment is constantly monitoring some of its observables [48]. This interaction induces *decoherence* (loss of coherence) of the system, that collapses into a state of the preferred basis; this process is otherwise called as *environment-induced superselection*, or *einselection*. It is important to notice that most scenarios lead to energy conservation which leads to the energy eigenbases being the preferred bases [3].

To illustrate, consider, for example, a system in contact with a thermal bath which is maintained at a certain constant temperature. After enough time, the system thermalizes with the bath, going to the thermal state

$$\rho = \frac{e^{-\beta H_S}}{Z},$$

where β is the inverse temperature of the bath, H_S is the system's Hamiltonian and Z is the partition function. It has no coherences in the energy basis of the system, and the energy eigenstates are the *einselected* states in this case.

For us to start quantifying coherence, it is necessary to make a small digression: it will be fundamental to present the concept of entropy in quantum information.

2.3   Von Neumann entropy

In information theory, be it classical or quantum, entropy is a key concept. In classical information theory, the *Shannon entropy* expresses information gain, that is, if you have a random variable X, when you learn its value, the entropy quantifies how much information you acquired [36]. The Shannon entropy depends only on the probabilities of the values that X may assume. Supposing it may assume the values $x_1, x_2, ..., x_N$ with probabilities $p_1, p_2, ..., p_N$, the definition is given by [36]

$$H(X) := -\sum_i p_i \log p_i.$$

The logarithm can be either base 2, which in commonly used in information theory, or base e, which is usually adopted in physics [39]. From now on, we will consider $\log$ to be in base e unless otherwise specified. As the function $x \log x$ is not defined for $x = 0$, when $p_i = 0$ we define $0 \log 0 \equiv 0$, in accordance to what we obtain when we take $\lim_{x \to 0} x \log x$ [36].

The quantum version of the Shannon entropy is the *von Neumann* entropy. Its definition is quite similar to the Shannon one, except that the probability distributions are replaced by density operators [36]. The definition of the von Neumann entropy is

$$S(\rho) := -\operatorname{tr}(\rho \log \rho) := -\sum_i \lambda_i \log \lambda_i, \tag{2.17}$$

where ρ is the quantum state and λ_i are its eigenvalues [36, 39].

In the same spirit as the Shannon entropy, the von Neumann entropy also expresses the information gained when we learn about the state of the system. Consider an arbitrary state $\rho = \sum_i \lambda_i |\psi_i\rangle\langle\psi_i|$. If ρ is a pure state, then all λ_i are zero except for one $\lambda_k = 1$. In this case, $S(\rho) = -1 \log 1 = 0$. That translates as: if the system is in a pure state, we already have all the information about it, so we have nothing to learn, and therefore the entropy is zero. That defines a lower bound for entropy, i.e.,

$$S(\rho) \geq 0. \tag{2.18}$$

On the other side, if ρ is the maximally mixed state $\rho = \mathbb{1}/d$ (as may be checked using the definition of purity in Eq. (2.3)) for a d-dimensional system, all its eigenvalues are the same, $\lambda_1 = \lambda_2 = ... = \lambda_N = 1/d$, and the entropy assumes its maximum value, $S(\rho) = \log(d)$ [39]. It is equally probable for the system to be in each of its eigenstates, so a priori we have no

information about it; upon measuring it, the system assumes a defined state, and information about it is acquired.

Another important property about entropy is that the entropy of a system does not change under unitary transformations, that is

$$S(U\rho\,U^\dagger) = S(\rho), \tag{2.19}$$

which may be derived using the fact that the trace is cyclic and the following property of unitaries: $f(U A\,U^\dagger) = U f(A)\,U^\dagger$. This implies that, as the time evolution of closed systems is represented by unitaries in quantum mechanics, entropy becomes a constant of motion [39].

2.3.1 Quantum relative entropy

Derived from von Neumann's entropy, we can build another important quantity for quantum information theory: the *quantum relative entropy*, or *Kullback-Leibler divergence* [49]. It is somewhat a measure of how distinguishable two states are; given two density operators ρ and σ, the relative entropy of ρ with respect to σ is defined by

$$S(\rho||\sigma) \coloneqq \operatorname{tr}(\rho\log\rho) - \operatorname{tr}(\rho\log\sigma) = -S(\rho) - \operatorname{tr}(\rho\log\sigma), \tag{2.20}$$

where, for the second equality, we have used the definition of von Neumann entropy in Eq. (2.17). The relative entropy is not symmetric, that is, $S(\rho||\sigma) \neq S(\sigma||\rho)$. Therefore, it cannot be considered a proper *distance* measure between two states, also because it does not satisfy the triangle inequality, i.e., the inequality $S(\rho||\sigma) \leq S(\rho||\gamma) + S(\gamma||\sigma)$ is not always valid [39]. Notwithstanding, it does satisfy *Klein's inequality*, that is,

$$S(\rho||\sigma) \geq 0, \tag{2.21}$$

with equality if and only if $\rho = \sigma$ [36].

2.4 Coherence quantifiers

Now that we are more familiar to the concepts of entropy and relative entropy, we return to the question of how to quantify coherence. For coherence quantifiers and a resource theory

of coherence to be defined, it is necessary to postulate which states are *incoherent* (i.e., not coherent) and which operations may be performed on these states such that they do not generate coherence [44]. As previously discussed, a state will be considered *incoherent* if is does not have off-diagonal elements in the *preferred basis* (Sec. 2.2). Considering a d-dimensional system with a certain preferred basis $\{|i\rangle\}$, any incoherent state will be diagonal in this basis, that is,

$$\delta = \sum_i \delta_i |i\rangle\langle i|, \tag{2.22}$$

where δ_i are the probabilities. These states form a set $\mathcal{I} \subset \mathcal{H}$, where $\mathcal{H}$ is the whole Hilbert space of the system. An *incoherent operation* is one which, by acting upon an incoherent state $\delta \in \mathcal{I}$, results another state $\delta' \in \mathcal{I}$ [44]. In addition, it may be deduced that the maximally coherent state is given by [44]

$$|\psi_{\mathrm{coh}}\rangle = \frac{1}{\sqrt{d}} \sum_i |i\rangle. \tag{2.23}$$

There is no unique form to quantify coherence; it is only necessary that a measure of coherence satisfies some constraints related to the states and operations we just presented. Any functional $\mathcal{C}$ that takes states into non-negative real numbers is a candidate for coherence quantifier if [44, 45]:

(C1) $\mathcal{C}(\delta) = 0$ if and only if $\delta \in \mathcal{I}$;

(C2) $\mathcal{C}(\rho) \geq \mathcal{C}(\Phi[\rho])$, for any incoherent operation Φ.

Those properties assure that incoherent states have no coherences, and incoherent operations do not increase the coherences of any state.

There are many possible monotones that respect the properties above. One example is the l_1 *norm of coherence* [44]. It is defined as

$$\mathcal{C}_{l_1}(\rho) = \sum_{\substack{i,j \\ i \neq j}} |\rho_{ij}|, \tag{2.24}$$

where $\rho_{ij} = \langle i|\rho|j\rangle$. This is a very intuitive and general measure, as coherence depends on the off-diagonal elements of a matrix. However, throughout this work, we will use another one: the *relative entropy of coherence*. The relative entropy of coherence is a distance-based quantifier of coherence [45] that considers as distance measure the quantum relative entropy. As we said, the relative entropy of coherence is not exactly a *distance*, but it expresses distinguishability

between two states. It also fulfils the conditions previously presented [44]. The relative entropy of coherence is defined as

$$\mathcal{C}(\rho) := \min_{\delta \in \mathcal{I}} S(\rho||\delta). \tag{2.25}$$

The minimization means the smallest distance from ρ to any incoherent state in $\mathcal{I}$. However, this expression can be rewritten as to avoid the need of minimization [45]. Considering a state $\delta = \sum_i \delta_i |i\rangle\langle i| \in \mathcal{I}$ and any state $\rho = \sum_{i,j} \rho_{ij} |i\rangle\langle j|$, we define $\Delta[\rho] := \sum_i \rho_{ii} |i\rangle\langle i|$ as the density operator containing only the diagonal entries of ρ. The relative entropy between ρ and δ is given by

$$S(\rho||\delta) = -S(\rho) - \mathrm{tr}(\rho \log \delta) = -S(\rho) - \mathrm{tr}(\Delta[\rho] \log \delta)$$

$$= S(\Delta[\rho]) - S(\rho) + S(\Delta[\rho]||\delta), \tag{2.26}$$

where we have used the property $\mathrm{tr}(\rho \log \delta) = \mathrm{tr}(\Delta[\rho] \log \delta)$ [45]. As the relative entropy is always positive, $S(\Delta[\rho]) - S(\rho) + S(\Delta[\rho]||\delta) \geq S(\Delta[\rho]) - S(\rho)$ and hence the minimum of $S(\rho||\delta)$ occurs for $\delta = \Delta[\rho]$ [39]. Consequently,

$$\mathcal{C}(\rho) = S(\Delta[\rho]) - S(\rho). \tag{2.27}$$

This shows that the relative entropy of coherence is actually just a difference in von Neumann entropies. This is generally not true for the relative entropy and it implies, in particular, that the relative entropy of coherence is bounded between 0 and $\log(d)$.

Chapter 3

Entropy production

The notion of entropy was first introduced in classical thermodynamics, related to the maximum heat exchanged between systems at definite temperatures [11,12]. In that context emerged the concept of *entropy production*; a closed system's entropy can never decrease under any transformation and, unless the process is reversible, it always increases. That is, besides posing a restriction on which transformations may be performed on physical systems, entropy production is also associated to irreversibility. Such as the concept of entropy itself, entropy production also appears in information theory, where it is related to the loss of information (as stated by *Landauer's principle* [1]).

With the emergence of quantum information as well as quantum thermodynamics, it became necessary to comprehend the role of entropy production in quantum processes and how the quantum aspects of a system may influence in its increase in entropy. In this chapter, we will review some features of entropy production in classical systems and present how it is defined and applied for quantum systems. In the quantum framework, we present in more detail the expression for entropy production in work protocols, and how to compute its stochastic version.

3.1   Classical systems

We begin by looking at entropy production from a thermodynamical point of view. Consider a system S interacting with multiple reservoirs at temperatures $T_1, T_2, ..., T_N$. The heat exchanged with the baths is, respectively, $Q_1, Q_2, ..., Q_N$, with Q_i positive if the heat is transferred from the environment to the system [12]. The change in system's entropy S_S is bounded

by [50]

$$\Delta S_S \geq \sum_i \frac{Q_i}{T_i}, \tag{3.1}$$

with the equality holding if and only if the process is reversible; i.e., in irreversible processes, entropy not only flows between system and reservoirs but is also generated within the system. That motivates the definition of the *entropy production* Σ as

$$\Sigma = \Delta S_S - \sum_i \frac{Q_i}{T_i} \geq 0. \tag{3.2}$$

Entropy production can also be expressed in terms of the work and free energy of the system if we consider a single reservoir [50]. The first law states that the change in the system's internal energy H_S is given by

$$\Delta H_S = Q - W, \tag{3.3}$$

where W represents the work done by the system. Also, the free energy is defined in terms of the internal energy and entropy as

$$F_S = H_S - TS_S. \tag{3.4}$$

If we now write $Q = \Delta H_S + W$ and substitute in Eq. (3.2), together with the fact that $\Delta F_S = \Delta H_S - T\Delta S_S$, we obtain

$$\Sigma = \beta(W - \Delta F_S), \tag{3.5}$$

where $\beta = 1/T$.

In information theory, irreversibility is crucial in understanding loss or erasure of information. For some information to be erased, Landauer's principle states that $\Delta S_S < 0$, i.e., $S_f < S_i$ [1], where $S_{f(i)}$ means the final (initial) entropy of the system. It may seem a bit counterintuitive at first, because according to what we previously stated about entropy, it seems that we would have more information in the end. That is true, except that the information we have is about the final state; we cannot acces information about the initial state anymore [50].

For concreteness, let us look at an example [10]. Consider the process depicted in Figure 3.1: a ball is placed on either left or right side of a box that is divided in half by a wall. The wall is then removed, allowing a piston to push the ball to the left corner of the box. Lastly, the piston is pulled back to its original position and the wall is reinserted. At the end, the ball will

always be on the left side, regardless of where it began.

We can represent this process as $P_{\text{left}} \left|\text{left}\right\rangle\left\langle\text{left}\right| + P_{\text{right}} \left|\text{right}\right\rangle\left\langle\text{right}\right| \rightarrow \left|\text{left}\right\rangle\left\langle\text{left}\right|$ [1]. With some probability P_{left} the ball starts on the left side of the box and with some other probability P_{right} it starts on the right side. If enough copies of this state are measured, the probabilities can be guessed and some information can be acquired about the state. Therefore, the entropy of the system at this point is non-zero. However, when the transformation occurs, the ball always ends up on the left side. So the entropy of the final state is zero, because there is no information gain upon measuring where the ball is. In spite of that, no information about the initial state can be acquired by measuring the final state. Thus, there was indeed loss of information and the change in entropy of the system is negative.
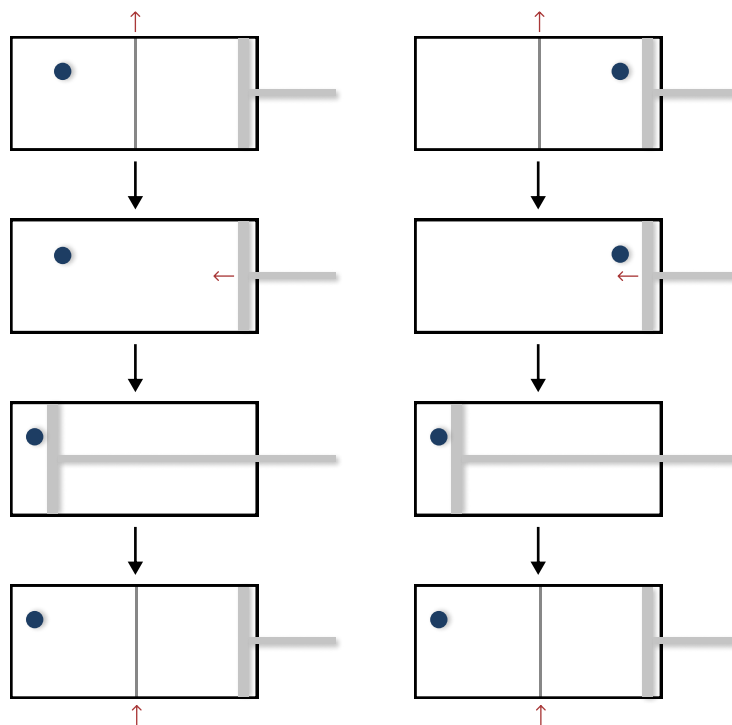
Figure 3.1: A schematic representation of information erasure: a ball is placed either on the left or on the right side of a box. It is then displaced by a piston and ends up on the left side regardless of where it began. At the end of the process, the information of the initial position of the ball was erased [10].

3.2 Quantum systems

In the quantum framework, entropy production arises when we talk about interactions between system and environment. Consider a system S and an environment E (of arbitrary di-

---

[1]Besides using the density matrix notation, notice that the process presented is entirely classical. States such as those indeed represent classical states, as noted in Sec. 2.1, as they have no quantum correlations.

mension) that begin in the product state $\rho_{SE} = \rho_S \otimes \rho_E$ and evolve globally according to the unitary U. Although it does not seem very general, a unitary evolution can encompass various types of interaction, from weak to strong couplings and time-dependent evolutions [50]. The evolved state of system plus environment is given by

$$\rho'_{SE} = U \rho_{SE} \, U^\dagger = U(\rho_S \otimes \rho_E) \, U^\dagger. \tag{3.6}$$

The final reduced state of the system can be obtained by taking the partial trace with respect to the environment, i.e.,

$$\rho'_S = \text{tr}_E(\rho'_{SE}) = \text{tr}_E \left\{ U(\rho_S \otimes \rho_E) \, U^\dagger \right\}. \tag{3.7}$$

As discussed in Sec. 2.1.1, tracing over the environment generates information loss, as the operation is irreversible. On the other hand, unitary operations do not change the system's entropy. Thus, the entropy production that takes place in the system can be linked to the fact that its correlations with the environment have been discarded and that we do not have access to any information about the bath anymore. Taking this into account, Ref. [51] has put forth a fully information theoretic definition of the entropy production, given by

$$\Sigma = \mathcal{I}_{\rho'_{SE}}(S : E) + S(\rho'_E || \rho_E), \tag{3.8}$$

where $\mathcal{I}_{\rho'_{SE}}(S : E) := S(\rho'_{SE} || \rho'_S \otimes \rho'_E) = S(\rho'_S) + S(\rho'_E) - S(\rho'_{SE})$ is the *mutual information* between system and environment, $S(\rho || \sigma)$ is defined in Eq. (2.20) and $\rho'_E = \text{tr}_S(\rho'_{SE})$ is the environment's final state [50, 51]. The mutual information between S and E expresses the information shared between them, which is lost when we trace over the environment. The second term is the relative entropy between the environment's final and initial state and represents the information lost about the environment itself. Eq. (3.8) is valid for any type of system and environment and any type of unitary interaction. It is also important to notice that, as we have already seen, the relative entropy is always non-negative, which implies that both terms in Σ are non-negative and so $\Sigma \geq 0$.

If we now rewrite the expression substituting the definition of mutual information and con-

sidering that $S(\rho||\sigma) = -S(\rho) - \text{tr}\{\rho \log \sigma\}$, we obtain

$$\Sigma = S(\rho_S') + S(\rho_E') - S(\rho_{SE}') - S(\rho_E') - \text{tr}\{\rho_E' \log \rho_E\}$$

$$= S(\rho_S') - S(\rho_S) - S(\rho_E) - \text{tr}\{\rho_E' \log \rho_E\}$$

$$= \Delta S_S + \text{tr}\{(\rho_E - \rho_E') \log \rho_E\}, \tag{3.9}$$

where we have used the fact that the entropy does not change under unitary operations and that the entropy of a product state is the sum of the individual entropies, and $\Delta S_S = S(\rho_S') - S(\rho_S)$ [50]. This form of the entropy production resembles the classical expression, Eq. (3.2), except that the second term is not necessarily related to heat flux. This term, in both classical and quantum cases, is associated to entropy flux.

3.2.1 Thermal environment and thermal operations

Considering the environment to be thermal, the second term in Eq. (3.9), related to changes in the environment, can indeed be related to heat [50]. Its initial state will be given by

$$\rho_E = e^{-\beta H_E}/Z_E, \tag{3.10}$$

where H_E is the environment's Hamiltonian and $Z_E = \text{tr}\{e^{-\beta H_E}\}$ is the partition function. By inserting this inside the logarithm of Eq. (3.9), we obtain

$$\Sigma = \Delta S_S + \text{tr}\{(\rho_E - \rho_E')(-\beta H_E - \log Z_E)\}$$

$$= \Delta S_S - \beta \text{tr}\{H_E(\rho_E - \rho_E')\}, \tag{3.11}$$

where we have used the fact that the trace of any density matrix is equal to one. The second term represents the energy change of the environment and can be associated to heat. However, this heat flux may not be the only energy change in the system, as the unitary may involve work as well [50]. The work done by the system can be defined in terms of the change in system's internal energy ΔH_S and the heat that leaves the environment $Q = \text{tr}\{H_E(\rho_E - \rho_E')\}$; it is defined as $W := Q - \Delta H_S$ [50]. Finally, by defining the *non-equilibrium free energy* as $F(\rho_S) = \text{tr}\{H_S \rho_S\} - TS(\rho_S)$, the entropy production in the quantum case can also be

expressed in terms of work and free energy as

$$\Sigma = \beta(W - \Delta F_S), \tag{3.12}$$

where $\Delta F_S = F(\rho'_S) - F(\rho_S)$.

A particular case of thermal environments is that of *thermal operations*. Those kinds of processes require a thermal environment and a *global fixed point*, that is, a state of the system $\bar{\rho}_S$ such that [50]

$$U(\bar{\rho}_S \otimes \rho_E)U^{\dagger} = \bar{\rho}_S \otimes \rho_E. \tag{3.13}$$

Both of these conditions insure that a thermal operation preserves the composite system's energy, i.e., $[U, H_S + H_E] = 0$. Taking that into account, the term related to entropy flux in Eq. (3.9), that usually depends on quantities related to the environment, can be rewritten in a way that it only depends on the system. The derivation, developed in [50], is presented in detail in Appendix A. The expression for the entropy production becomes

$$\Sigma = S(\rho_S||\rho_S^{th}) - S(\rho'_S||\rho_S^{th}). \tag{3.14}$$

We can interpret the expression above as comparing how far away from thermal equilibrium the initial and final states of the system (ρ_S and ρ'_S) are. Entropy production, on top of being related to irreversibility, is related to far from equilibrium processes. If we go back to classical thermodynamics, a reversible process can be associated to adiabaticity (in the classical sense of the word). An adiabatic process is one that occurs without heat transfer between system and environment. For this to be true, the system's state cannot be pushed far from thermal equilibrium. This holds for quantum systems as well. When a system undergoes a transformation that takes it to a state far from equilibrium, the transformation is irreversible and there is entropy production involved.

Thermal operations are still a very vast and important class of processes, in spite of being easier to deal with as the entropy production only depends on the system's states. Therefore, in this work we will be interested mainly on these operations. All derivations that follow will assume the entropy production as expressed in Eq. (3.14).

3.2.2 Work protocols

Inside the thermal operations' class of processes, we will look at *work protocols*. Consider a system S that begins in the thermal state $\rho_i^{th} = e^{-\beta H_i}/Z_i$ (where H_i is the system's initial Hamiltonian and Z_i is the partition function) in equilibrium with a bath at inverse temperature β. Suppose it is possible to change an external parameter $\lambda(t)$ such that it changes the Hamiltonian [52,53]. A work protocol is implemented by changing the parameter, taking $H_i = H(\lambda(0))$ to $H_f = H(\lambda(\tau))$, where τ is the protocol's duration [50]. The evolution of the system is given by the unitary $U = e^{-iH(\lambda(t))t}$ and the final state of the system is $\rho_\tau = U\rho_i^{th}U^\dagger$. At the end, the system is allowed to thermalize in contact with the bath, reaching the state $\rho_f^{th} = e^{-\beta H_f}/Z_f$. The protocol is depicted in Figure 3.2.

Figure 3.2: Representation of a work protocol: a system is initially in state ρ_i^{th}, in thermal equilibrium with a bath with energy H_i. An external parameter is changed such that it drives the system to a non-equilibrium state ρ_τ through a unitary protocol (given by the unitary U) and changes the bath's Hamiltonian to H_f. Afterwards, the system is allowed to relax, again in contact with the bath and reaches the thermal state ρ_f^{th}. Alternatively, the system could go from state ρ_i^{th} to ρ_f^{th} by a quasi-static process such that it is never far from equilibrium.

The entropy produced during the protocol stems from the final thermalization step, as the unitary evolution does not change the entropy of the system. Therefore, as the final state of the system is already the thermal state, the second term on Eq. (3.14) vanishes and the entropy production will be given by

$$\Sigma = S(\rho_\tau || \rho_f^{th})$$
$$= \text{tr}\left\{\rho_\tau \log \rho_\tau - \rho_\tau \log \rho_f^{th}\right\}$$
$$= -S(\rho_\tau) - \text{tr}\left\{\rho_\tau \log \rho_f^{th}\right\}. \qquad (3.15)$$

Notwithstanding, the entropy production can be associated to the unitary evolution itself [50]. As stated before, thermal operations are non-equilibrium processes; that is, the evolution takes the system to a state far from thermal equilibrium. If the system was maintained at a thermal state during the whole protocol, i.e., if the evolution was quasi-static (depicted in Figure 3.2 by the bottom arrow), no entropy production would arise. So, the entropy production could be defined simply by comparing the implemented protocol with an ideal quasi-static one, without even mentioning the final step of thermalization.

3.2.3   Fluctuation theorems and stochastic trajectories

So far we have discussed entropy production in the average sense. Now we will deal with stochastic trajectories and fluctuation theorems for the entropy production. The following deductions are based solely on work protocols as defined in Sec. 3.2.2.

Let the initial energy basis be $H_i = \sum_n \epsilon_n^i |n\rangle\langle n|$. The protocol is implemented considering the *two-point measurement* (TPM) scheme [6]: first, we measure ρ_i^{th} in the initial eigenbasis. The probability of obtaining a specific state $|n\rangle$ is $p_n^i = e^{-\beta\epsilon_n^i}/Z_i$. Then, we apply the unitary $U = e^{-iH(t)t}$ to the state $|n\rangle$, obtaining $U|n\rangle$. Finally, we measure the state in the energy basis $\{|m'\rangle\}$ of the final Hamiltonian $H_f = \sum_{m'} \epsilon_{m'}^f |m'\rangle\langle m'|$. The Hamiltonians $H_i = H(0)$, $H(t)$ and $H_f = H(\tau)$ come from the change of the external parameter $\lambda(t)$ aforementioned. They are, in general, different and have incompatible eigenbasis.

The probability of obtaining the state $|m'\rangle$ given that the initial state was $|n\rangle$ is given by

$$p_{m'|n} = |\langle m'|U|n\rangle|^2. \tag{3.16}$$

We define the joint probability of obtaining $|n\rangle$ and $|m'\rangle$, or else the probability of the quantum trajectory $\zeta = \{n, m'\}$, as

$$P[\zeta] = P[n, m'] = p_{m'|n}\, p_n^i. \tag{3.17}$$

To compute the entropy production, we need to consider that an irreversible process cannot be perfectly reversed, by definition, but a corresponding backward process can be associated to it (in fact, the backward process does not even need to be unique [50]). As an intuitive example, Jarzynski suggests [37] that we consider a rubber band: after it is stretched, it can be contracted, but the reversed process is asymmetric because of alterations suffered by the material. The work done to stretch the rubber band is greater than the one done to contract it,

because part of the work is irretrievably lost. In microscopic processes such as the ones we are interested in, when considering a specific stochastic trajectory, the entropy produced can be recovered by comparing the forward and corresponding backward process. This is done by taking into account *Crooks's fluctuation theorem* [53], that states that

$$\frac{P_F[\zeta_F]}{P_B[\zeta_B]} = e^{\sigma}, \tag{3.18}$$

where $P_{F(B)}[\zeta_{F(B)}]$ is the forward (backward) probability of the forward (backward) trajectory $\zeta_{F(B)}$, and σ is the stochastic entropy production. It is important to notice that Crooks's relation directly implies that there is a *Jarzynski's equality* [52] for σ, that is, $\langle e^{-\sigma} \rangle = 1$.

Returning to the process of interest, the reversed trajectory is as follows: the system starts in state ρ_f^{th} and is measured in the eigenbasis of H_f, resulting in $|m'\rangle$ with probability $p_{m'}^f = e^{-\beta \epsilon_{m'}^f}/Z_f$. Then, it undergoes an evolution given by $U^\dagger$ and reaches state $|n\rangle$ with probability $p_{n|m'} = |\langle n|U^\dagger|m'\rangle|^2 = p_{m'|n}$. The probability of a trajectory $\zeta_B = \{m', n\}$ is given by

$$P_B[\zeta_B] = P[m', n] = p_{n|m'}\, p_{m'}^f = p_{m'|n}\, p_{m'}^f. \tag{3.19}$$

Finally, with $P_F[\zeta_F]$ given by Eq. (3.17), the stochastic entropy production is given by

$$\sigma[n, m'] = \log \frac{P_F[\zeta_F]}{P_B[\zeta_B]} = \log p_n^i - \log p_{m'}^f. \tag{3.20}$$

We may check that its average indeed corresponds to Σ defined in Eq. (3.15). The mean value of the entropy production is

$$
\begin{aligned}
\langle \sigma[n, m'] \rangle &= \sum_{n, m'} P[n, m']\sigma[n, m'] \\
&= \sum_{n, m'} p_{m'|n}\, p_n^i (\log p_n^i - \log p_{m'}^f) \\
&= \sum_n \left[\left(\sum_{m'} p_{m'|n} \right) p_n^i \log p_n^i \right] - \sum_{m'} \left[\left(\sum_n p_{m'|n}\, p_n^i \right) \log p_{m'}^f \right].
\end{aligned}
$$

Now, we consider two important identities:

$$\sum_{m'} p_{m'|n} = \sum_{m'} \langle n|U^\dagger|m'\rangle\, \langle m'|U|n\rangle = \langle n| U \left(\sum_{m'} |m'\rangle\langle m'| \right) U^\dagger |n\rangle = 1, \tag{3.21}$$

and

$$\sum_n p_{m'|n} \, p_n^i = \langle m'| U \left(\sum_n p_n^i \, |n\rangle\langle n| \right) U^\dagger \, |m'\rangle = \langle m'| U \rho_i^{th} U^\dagger |m'\rangle = \langle m'| \rho_\tau |m'\rangle. \quad (3.22)$$

Therefore,

$$\langle \sigma[n, m'] \rangle = \sum_n p_n^i \log p_n^i - \sum_{m'} \langle m'| \rho_\tau |m'\rangle \log p_{m'}^f$$

$$= \operatorname{tr}\big(\rho_i^{th} \log \rho_i^{th}\big) - \operatorname{tr}\big(\rho_\tau \log \rho_f^{th}\big)$$

$$= S(\rho_\tau || \rho_f^{th}) = \Sigma. \quad (3.23)$$

Thus, Eq. (3.20) can indeed represent the stochastic entropy production. We can also substitute in it the definitions for the thermal populations $p_n^i = e^{-\beta \epsilon_n^i}/Z_i$ and $p_{m'}^f = e^{-\beta \epsilon_{m'}^f}/Z_f$, which results in

$$\sigma[n, m'] = \beta(\epsilon_{m'}^f - \epsilon_n^i) - \beta \Delta F, \quad (3.24)$$

where $\Delta F = F_f - F_i$ is the difference between the final and initial Helmholtz's free energies $F_{f(i)} = -T \log Z_{f(i)}$. The first interesting thing to notice is that σ is not necessarily positive. For example, if we take $H_f = H_i$ such that $\Delta F = 0$, we would have $\epsilon_m^f = \epsilon_m^i \equiv \epsilon_m$ and so $\sigma[n, m] = \beta(\epsilon_m - \epsilon_n)$. In general, there would be as negative as positive values of $\sigma[n, m]$: if $\epsilon_k > \epsilon_\ell$, we would have $\sigma[\ell, k] > 0$ and $\sigma[k, \ell] < 0$. However, the probabilities of the negative contributions are smaller, such that, in average, the entropy production is always positive, as we have already seen in the beginning of this chapter.

For completeness, we also compute the variance $\operatorname{Var}(\sigma) = \langle \sigma^2 \rangle - \langle \sigma \rangle^2$. First, $\langle \sigma^2 \rangle$ is given by

$$\langle \sigma^2 \rangle = \sum_{n,m'} P[n, m'] \, \sigma[n, m']^2$$

$$= \sum_{n,m'} p_{m'|n} \, p_n^i \left(\log p_n^i - \log p_{m'}^f \right)^2. \quad (3.25)$$

We could stop here and write the variance as

$$\operatorname{Var}(\sigma) = \sum_{n,m'} p_{m'|n} \, p_n^i \left(\log p_n^i - \log p_{m'}^f \right)^2 - \left[\sum_{n,m'} p_{m'|n} \, p_n^i \left(\log p_n^i - \log p_{m'}^f \right) \right]^2, \quad (3.26)$$

but let us proceed and write it as well in terms of traces of density matrices. Proceeding with the first term, we get

$$\langle \sigma^2 \rangle = \sum_{n,m'} p_{m'|n}\, p_n^i \left[(\log p_n^i)^2 + (\log p_{m'}^f)^2 - 2\log p_n^i \log p_{m'}^f \right]$$

$$= \sum_{n,m'} p_{m'|n}\, p_n^i (\log p_n^i)^2 + \sum_{n,m'} p_{m'|n}\, p_n^i (\log p_{m'}^f)^2 - 2\sum_{n,m'} p_{m'|n}\, p_n^i \log p_n^i \log p_{m'}^f.$$

Summing the first term in m' and the second in n, we obtain

$$\langle \sigma^2 \rangle = \sum_{n} p_n^i (\log p_n^i)^2 + \sum_{m'} p_{m'}^f (\log p_{m'}^f)^2 - 2\sum_{n,m'} p_{m'|n}\, p_n^i \log p_n^i \log p_{m'}^f. \tag{3.27}$$

The first two terms are trivially written in terms of density operators, but for the last term we will make use of the definition $p_{m'|n} = |\langle m'|U|n\rangle|^2$.

$$\sum_{n,m'} p_{m'|n}\, p_n^i \log p_n^i \log p_{m'}^f = \sum_{n,m'} |\langle m'|U|n\rangle|^2\, p_n^i \log p_n^i \log p_{m'}^f$$

$$= \sum_{n,m'} \langle m'| \log\!\big(\rho_f^{th}\big)\, U\, \rho_i^{th} \log \rho_i^{th} |n\rangle\langle n| U^\dagger |m'\rangle$$

$$= \mathrm{tr}\left\{ \log\!\big(\rho_f^{th}\big)\, \rho_\tau \log \rho_\tau \right\}. \tag{3.28}$$

Finally, we have

$$\langle \sigma^2 \rangle = \mathrm{tr}\left\{ \rho_i^{th} (\log \rho_i^{th})^2 \right\} + \mathrm{tr}\left\{ \rho_f^{th} (\log \rho_f^{th})^2 \right\} - 2\,\mathrm{tr}\left\{ \log\!\big(\rho_f^{th}\big)\, \rho_\tau \log \rho_\tau \right\},$$

$$\tag{3.29}$$

and

$$\langle \sigma \rangle^2 = \left(\mathrm{tr}\left\{ \rho_i^{th} \log \rho_i^{th} \right\} - \mathrm{tr}\left\{ \rho_f^{th} \log \rho_f^{th} \right\} \right)^2, \tag{3.30}$$

so the variance is given by $\mathrm{Var}(\sigma) = \langle \sigma^2 \rangle - \langle \sigma \rangle^2$, with $\langle \sigma^2 \rangle$ and $\langle \sigma \rangle^2$ given by Eqs. (3.29) and (3.30).

3.2.4   Limiting cases for stochastic entropy production in work protocols

We have reached general expressions for the stochastic entropy production, its probability distribution and average. However, if we want to understand how they depend on the system's

parameters (such as dimension and the time period that the system is driven out of equilibrium), we have to solve for the eigenvalues and eigenvectors of the initial and final Hamiltonians, which is not always an easy task. In fact, it cannot be done analytically depending on the model applied and the dimension of the system. Therefore, to gain some intuition before we present some numerical results, we propose two limit cases that represent interesting physical processes and that enable us to achieve some analytical results.

$H_f = H_i$ and small τ

The first interesting case we can analyse is that of a very quick change in the external parameter: the Hamiltonian is quenched from H_i to H by a small period of time τ and then quenched back to the original Hamiltonian ($H \to H_i$). Assuming a small τ, we may expand the unitary until order τ^2, that is $U = \exp\{-iH\tau\} \approx 1 - iH\tau - H^2\tau^2/2$. As the initial and final Hamiltonian are the same, they share the same eigenbasis $\{|n\rangle\}$ and we can rewrite $\epsilon_{m'}^f = \epsilon_m^i \equiv \epsilon_m$. Also, the final and initial populations of the corresponding thermal states are the same: $p_{m'}^f = p_m^i$. So, in Eq. (3.24), $\Delta F = 0$, as $Z_f = Z_i$, and then

$$\sigma[n, m] = \beta(\epsilon_m - \epsilon_n). \tag{3.31}$$

To see how the entropy production behaves in average, let us rewrite the expression for the probabilities $P[n, m] = p_{m|n}\, p_n^i$, $p_{m|n} = |\langle m|U|n\rangle|^2$. We have

$$\langle m|U|n\rangle \approx \langle m| \left(1 - iH\tau - \frac{H^2\tau^2}{2} \right) |n\rangle$$

$$= \delta_{mn} - i\tau \langle m|H|n\rangle - \frac{\tau^2}{2} \langle m|H^2|n\rangle, \tag{3.32}$$

and so

$$|\langle m|U|n\rangle|^2 \approx \delta_{mn} + i\tau\big(\delta_{mn} \langle n|H|m\rangle - \delta_{mn} \langle m|H|n\rangle\big) + \tau^2\big(|\langle m|H|n\rangle|^2$$

$$-\frac{1}{2}\delta_{mn} \langle n|H^2|m\rangle - \frac{1}{2}\delta_{mn} \langle m|H^2|n\rangle\big) + \mathcal{O}(\tau^3)$$

$$= \delta_{mn} + \tau^2\big(|\langle m|H|n\rangle|^2 - \delta_{mn} \langle n|H^2|n\rangle\big). \tag{3.33}$$

Therefore, $P[n, m]$ is given by

$$P[n, m] = \delta_{mn}\, p_n^i + \tau^2\, p_n^i \left(| \langle m|H|n \rangle |^2 - \delta_{mn} \langle n|H^2|n \rangle \right). \tag{3.34}$$

At last, the average entropy production is given by

$$
\begin{aligned}
\Sigma = \langle \sigma \rangle &= \beta \sum_{n,m} \sigma[n, m]\, p[n, m] \\
&= \sum_{n,m} \left[\delta_{nm}\, p_n^i (\epsilon_m - \epsilon_n) + \tau^2 p_n^i (\epsilon_m - \epsilon_n)(| \langle m|H|n \rangle |^2 - \delta_{nm} \langle n|H^2|n \rangle) \right] \\
&= \beta\tau^2 \sum_{n,m} p_n^i (\epsilon_m - \epsilon_n)\, | \langle m|H|n \rangle |^2,
\end{aligned}
\tag{3.35}
$$

where we have used the fact that $\delta_{nm}(\epsilon_m - \epsilon_n) = 0$.

It is interesting to notice that, in this case, we can easily find a general expression for any cumulant of the distribution of entropy production. Considering the j-th cumulant $\kappa_j(\sigma) = \langle (\sigma - \langle \sigma \rangle)^j \rangle$, the first term of the expansion will always be $\langle \sigma^j \rangle = \sum_{n,m} \sigma[n, m]^j P[n, m]$, that is, the j-th moment. Substituting Eq. (3.31) and opening the expression, we obtain

$$
\begin{aligned}
\sigma[n, m]^j\, P[n, m] = {} & \beta^j \delta_{mn}\, p_n^i\, (\epsilon_m - \epsilon_n)^j + \beta^j \tau^2\, p_n^i (\epsilon_m - \epsilon_n)^j \left(| \langle m|H|n \rangle |^2 \right. \\
& \left. - \delta_{mn} \langle n|H^2|n \rangle \right).
\end{aligned}
\tag{3.36}
$$

All the terms with $\delta_{mn}(\epsilon_m - \epsilon_n)^j$ will vanish, and we will remain with

$$\sigma[n, m]^j\, P[n, m] = \beta^j \tau^2 p_n^i (\epsilon_m - \epsilon_n)^j | \langle m|H|n \rangle |^2. \tag{3.37}$$

As for the other terms of $\kappa_j(\sigma)$, they will depend on a multiplication of moments of σ. But, as we have just seen, all the moments are proportional to τ^2, and by multiplying two or more of them, we obtain higher orders on τ, which will not be relevant for the problem we are dealing with. As a result, we conclude that

$$\kappa_j(\sigma) = \beta^j \tau^2 \sum_{n,m} p_n^i\, (\epsilon_m - \epsilon_n)^j | \langle m|H|n \rangle |^2. \tag{3.38}$$

As we see from Eq. (3.38), as long as time τ is small, the time dependence for all cumulants is the same. On the other hand, the dependence on β grows exponentially with the order of the

cumulant.

$H_f = H_i + \delta H$ and $\tau \to 0, U = 1$

Now, we want to see what happens when we add a little perturbation to the initial Hamiltonian such that the final Hamiltonian is given by $H_f = H_i + \delta H$, where $\delta H \ll H_i$. The perturbation will imply that the bases that diagonalize the initial and final Hamiltonians are different, and therefore we will use perturbation theory to calculate the eigenvectors of H_f [54]. Moreover, we will study the scenario of an instantaneous quench, that is, $\tau \to 0$, and so the unitary becomes trivial ($U \to 1$).

Let $\{|n\rangle\}$ be the basis of H_i and $\{|n'\rangle\}$ the basis of H_f, with each state $|n'\rangle$ being a perturbed version of the correspond state $|n\rangle$ of the initial basis. The initial and final states are respectively $\rho_i^{th} = \sum_n p_n^i |n\rangle\langle n|$ and $\rho_\tau = U\rho_i^{th}U^\dagger = \rho_i^{th}$.

The stochastic entropy production is given by

$$\sigma[n, m'] = \log p_n^i - \log p_{m'}^f = \beta(\epsilon_{m'}^f - \epsilon_n^i) - \beta\Delta F, \tag{3.39}$$

where the perturbed eigenenergies $\epsilon_{m'}$ up to $\mathcal{O}(\delta H^2)$ are given by [54]

$$\epsilon_{m'}^f = \epsilon_m^i + \langle m|\delta H|m\rangle + \sum_{k\neq m} \frac{|\langle k|\delta H|m\rangle|^2}{\epsilon_m^i - \epsilon_k^i}. \tag{3.40}$$

To compute the average entropy production and other cumulants, we need to write the probabilities $P[n, m']$. We start by noting that the eigenvectors of H_f are given by

$$|m'\rangle = \left|m'^{(0)}\right\rangle + \left|m'^{(1)}\right\rangle + \left|m'^{(2)}\right\rangle + \mathcal{O}(\delta H^3), \tag{3.41}$$

with [54]

$$\left|m'^{(0)}\right\rangle = |m\rangle, \tag{3.42}$$

$$\left|m'^{(1)}\right\rangle = \sum_{k\neq m} \frac{\langle k|\delta H|m\rangle}{\epsilon_m^i - \epsilon_k^i} |k\rangle, \tag{3.43}$$

$$\left|m'^{(2)}\right\rangle = \sum_{k\neq m}\sum_{\ell\neq m} \frac{\langle k|\delta H|\ell\rangle\,\langle\ell|\delta H|m\rangle}{(\epsilon^i_m - \epsilon^i_k)(\epsilon^i_m - \epsilon^i_\ell)}\,|k\rangle - \sum_{k\neq m} \frac{\langle m|\delta H|m\rangle\,\langle k|\delta H|m\rangle}{(\epsilon^i_m - \epsilon^i_k)^2}\,|k\rangle$$

$$-\frac{1}{2}\sum_{k\neq m} \frac{\langle m|\delta H|k\rangle\,\langle k|\delta H|m\rangle}{(\epsilon^i_m - \epsilon^i_k)^2}\,|m\rangle. \tag{3.44}$$

Next, we will look at the transition probability from a state $|n\rangle$ to $|m'\rangle$, $p_{m'|n} = |\langle m'|U|n\rangle|^2$. The matrix element $\langle m'|U|n\rangle$ is given by

$$\langle m'|U|n\rangle \approx \langle m'|n\rangle \approx \delta_{mn} + \sum_{k\neq m}\frac{\langle m|\delta H|k\rangle}{\epsilon^i_m - \epsilon^i_k}\delta_{nk} + \sum_{k\neq m}\sum_{\ell\neq m}\frac{\langle\ell|\delta H|k\rangle\,\langle m|\delta H|\ell\rangle}{(\epsilon^i_m - \epsilon^i_k)(\epsilon^i_m - \epsilon^i_\ell)}\delta_{nk}$$

$$-\sum_{k\neq m}\frac{\langle m|\delta H|m\rangle\,\langle m|\delta H|k\rangle}{(\epsilon^i_m - \epsilon^i_k)^2}\delta_{nk} - \frac{1}{2}\sum_{k\neq m}\frac{\langle k|\delta H|m\rangle\,\langle m|\delta H|k\rangle}{(\epsilon^i_m - \epsilon^i_k)^2}\delta_{mn} + \mathcal{O}(\delta H^3). \tag{3.45}$$

Let us separate now in two cases: $m = n$ and $m \neq n$. In the case where $m = n$, the second, third and fourth terms of the expression above vanish, so the matrix element is given by

$$\langle n'|U|n\rangle = 1 - \frac{1}{2}\sum_{k\neq n}\frac{|\langle n|\delta H|k\rangle|^2}{(\epsilon^i_n - \epsilon^i_k)^2}. \tag{3.46}$$

When $m \neq n$, however, the first and fifth terms vanish and the result becomes

$$\langle m'|U|n\rangle = \frac{\langle m|\delta H|n\rangle}{\epsilon^i_m - \epsilon^i_n} + \sum_{\ell\neq m}\frac{\langle\ell|\delta H|n\rangle\,\langle m|\delta H|\ell\rangle}{(\epsilon^i_m - \epsilon^i_n)(\epsilon^i_m - \epsilon^i_\ell)} - \frac{\langle m|\delta H|m\rangle\,\langle m|\delta H|n\rangle}{(\epsilon^i_m - \epsilon^i_n)^2}. \tag{3.47}$$

Now, for the probabilities of transition themselves, up until $\mathcal{O}(\delta H^2)$ we have,

$$p_{m'|n} = \begin{cases} 1 - \displaystyle\sum_{k\neq n}|h_{nk}|^2, & \text{for } m = n, \\[2mm] |h_{mn}|^2, & \text{for } m \neq n, \end{cases} \tag{3.48}$$

where

$$|h_{ab}|^2 = \frac{|\langle a|\delta H|b\rangle|^2}{(\epsilon^i_a - \epsilon^i_b)^2}. \tag{3.49}$$

Just for a sanity check, let us suppose that the perturbation δH is zero. In this case, the initial and final Hamiltonians and therefore their eigenbases are the same. As we are considering the quench to be instantaneous, it means that the system state remains the same. In Eq. (3.46), the

second term would vanish, which means that the probability of obtaining the same state after the unitary (which does nothing) is applied is 1, while, taking a look at Eq. (3.47), as all terms depend on δH, the probability of obtaining a different state is zero. This is exactly what we would expect.

We could try another sanity check. If we take the probabilities $p_{m'|n}$ for $m \neq n$ and sum over $m \neq n$, and then sum with the probability for $m = n$ (that is, we are summing over all possible m), the terms that are quadratic in δH cancel and we get 1, which is the expected result, as the probability of getting any state given that the initial state is $|n\rangle$ is 1.

Finally, we have all the tools to compute the cumulants of the entropy production. The average entropy production is given by

$$
\Sigma = \langle \sigma \rangle = \sum_{n,m'} \sigma[n,m'] \, P[n,m']
$$

$$
= \beta \sum_n p_n^i \left\{ \left(1 - \sum_{k \neq n} |h_{nk}|^2 \right) [(\epsilon_{n'}^f - \epsilon_n^i) - \Delta F] + \sum_{m \neq n} |h_{mn}|^2 \, [(\epsilon_{m'}^f - \epsilon_n^i) - \Delta F] \right\}
$$

$$
= \beta \sum_n p_n^i \left\{ (\epsilon_{n'}^f - \epsilon_n^i) - \Delta F - (\epsilon_{n'}^f - \epsilon_n^i) \sum_{k \neq n} |h_{nk}|^2 + \Delta F \sum_{k \neq n} |h_{nk}|^2 \right.
$$

$$
\left. + \sum_{m \neq n} |h_{mn}|^2 (\epsilon_{m'}^f - \epsilon_n^i) - \Delta F \sum_{m \neq n} |h_{mn}|^2 \right\}.
$$

As $|h_{mn}|^2 = |h_{nm}|^2$ and m is an arbitrary index in the last sum, we can replace the sum by $\sum_{k \neq n} |h_{nk}|^2$ and cancel it with the fourth term. Then, collecting the remaining terms,

$$
\Sigma = \beta \sum_n p_n^i \left\{ (\epsilon_{n'}^f - \epsilon_n^i) - \Delta F - (\epsilon_{n'}^f - \epsilon_n^i) \sum_{k \neq n} |h_{nk}|^2 + \sum_{m \neq n} |h_{mn}|^2 (\epsilon_{m'}^f - \epsilon_n^i) \right\}
$$

$$
= \beta \sum_n p_n^i \left\{ (\epsilon_{n'}^f - \epsilon_n^i) - \Delta F + \sum_{m \neq n} |h_{mn}|^2 (\epsilon_{m'}^f - \epsilon_{n'}^f) \right\}. \tag{3.50}
$$

We can now substitute the eigenvalues of the final Hamiltonian for the expression in Eq. (3.40). We notice that, in the last term of the expression above, the terms of $\epsilon_{m'}^f$ and $\epsilon_{n'}^f$ which depend on any order of δH will become of $\mathcal{O}(\delta H^3)$ when multiplied by $|h_{mn}|^2$. We will disregard this

terms, as we are interested in small δH. The expression then becomes

$$\Sigma = \beta \sum_n p_n^i \left\{ \langle n|\delta H|n \rangle + \sum_{k \neq n} \frac{|\langle k|\delta H|n \rangle|^2}{\epsilon_n^i - \epsilon_k^i} + \sum_{m \neq n} |h_{mn}|^2 (\epsilon_m^i - \epsilon_n^i) - \Delta F \right\}$$

$$= \beta \sum_n p_n^i \left\{ \langle n|\delta H|n \rangle + \sum_{k \neq n} \frac{|\langle k|\delta H|n \rangle|^2}{\epsilon_n^i - \epsilon_k^i} + \sum_{m \neq n} \frac{|\langle m|\delta H|n \rangle|^2}{(\epsilon_m^i - \epsilon_n^i)^2} (\epsilon_m^i - \epsilon_n^i) - \Delta F \right\}$$

$$= \beta \sum_n p_n^i \left\{ \langle n|\delta H|n \rangle + \sum_{k \neq n} \frac{|\langle k|\delta H|n \rangle|^2}{\epsilon_n^i - \epsilon_k^i} - \sum_{m \neq n} \frac{|\langle m|\delta H|n \rangle|^2}{\epsilon_n^i - \epsilon_m^i} - \Delta F \right\}. \tag{3.51}$$

Again, the indices k and m in the second and third terms are arbitrary, so these terms cancel. Also, in the last term, ΔF can be taken out of the sum, as it does not depend on n, and the sum over n of the probabilities p_n^i is equal to 1. The final expression is

$$\Sigma = \beta \sum_n p_n^i \langle n|\delta H|n \rangle - \beta \Delta F$$

$$= \beta \left[\text{tr} \left(\rho_i^{th} \delta H \right) - \Delta F \right]$$

$$= \beta \left[\text{tr}(\rho_\tau H_f) - \text{tr} \left(\rho_i^{th} H_i \right) - \Delta F \right]. \tag{3.52}$$

We point out that the analysis we can do without specifying a real physical model is limited. Therefore, we shall proceed to present the models to which we will apply the theory developed.

Chapter 4

Models

The main objective of this dissertation is to analyse how coherence contributes to stochastic entropy production in work protocols. For that end, we will apply the theory that will be presented in Chapters 5 and 6 to two different models: a macrospin and the Lipkin-Meshkov-Glick (LMG) model [7–9]. Both of these models represent systems of multiple particles that behave as a collective unique spin. They therefore have the characteristic of having a tunable dimensionality. That is an interesting feature, as it allows us to perceive if they behave as we would expect for larger dimensions (i.e., according to classical thermodynamics' laws).

In this chapter, we present both models and expose some results of how stochastic entropy production [Eq. (3.20)] behaves in each of them for a minimal qubit example.

We note that, for simplicity, the external parameter involved in the work protocol (Fig. 3.2) will have no time dependence ($\lambda(t) \equiv \lambda$). This implies that the evolution will be composed of quenches: the Hamiltonian instantaneously changes from H_i to H and then, after a time period τ, it changes instantaneously from H to H_f.

4.1 Macrospin model

Before we present the model itself, we should briefly review some important properties of spin operators. The operators S_x, S_y and S_z are the components of the spin $\boldsymbol{S}$ into the x, y and z axes. They obey the commutation relations of angular momentum, that is, $[S_i, S_j] = i\, \varepsilon_{ijk}\, S_k$, where ε_{ijk} is the *Levi-Civita tensor* [54,55]. The eigenvectors of S_z obey the following property:

$$S_z \left| S\, m \right\rangle = m \left| S\, m \right\rangle, \tag{4.1}$$

where S is the total spin and $m = -S, -S+1, ..., S-1, S$. The basis of S_z is set to be the canonical basis. From the eigenvectors of S_z, we can derive the matrix elements of S_x and S_y. We have that

$$\langle S'\, m' |\, S_\pm\, | S\, m \rangle = \sqrt{S(S+1) - m(m \pm 1)}\delta_{S,S'}\delta_{m',m'\pm 1}, \tag{4.2}$$

with $S_x = (S_+ + S_-)/2$, $S_y = (S_+ - S_-)/2i$ [56]. Now, onto the model itself.

The macrospin model consists of a collective spin of dimension $d = 2S + 1$, with spin operators S_x, S_y, S_z, that starts in equilibrium, aligned in the z-direction. It is taken away from equilibrium by means of a magnetic pulse in the transverse (x) direction. At the end, the system is allowed to thermalize again. It is a simple model, that can be analytically solved for a 2-dimensional system (qubit).

The system begins in the thermal state of the initial Hamiltonian $H_i = -h_z S_z = \sum_{n=0}^{d-1} \epsilon_n^i |n\rangle\langle n|$, where $\epsilon_n^i = -S, -S+1, ..., S-1, S$. That is,

$$\rho_i^{th} = \frac{e^{-\beta H_i}}{Z_i} = \sum_n p_n^i |n\rangle\langle n|, \tag{4.3}$$

where $p_n^i = e^{-\beta \epsilon_n}/Z_i$, $Z_i = \text{tr}\{e^{-\beta H_i}\}$ is the partition function. We follow with the two-point measurement (TPM) scheme [6]: the system is then measured in the initial energy basis, giving an outcome $|n\rangle$ with probability p_n^i. Afterwards, the magnetic pulse in the x-direction is applied and the system evolves unitarily for a fixed time-period τ, with $U = e^{-iH\tau}$, where

$$H = H_i - h_x S_x = -h_z S_z - h_x S_x. \tag{4.4}$$

The final state, $\rho_\tau = U \rho_i^{th} U^\dagger$, is at last measured in the energy basis of the final Hamiltonian H_f. At this point, the final Hamiltonian could be arbitrary, but we will consider, for simplicity, that it is reinitialized such that $H_f = H_i$. The outcome of the final measurement is given by a state $|m\rangle$ with probability p_m^τ.

As the initial and final bases are the same, $\rho_f^{th} = \rho_i^{th}$ and the stochastic entropy production

will be given, according to Eq. (3.20), by

$$\sigma[n, m] = \log p_n^i - \log p_m^i$$

$$= \log \left(e^{-\beta \epsilon_n} / Z_i \right) - \log \left(e^{-\beta \epsilon_m} / Z_i \right)$$

$$= \beta(\epsilon_m - \epsilon_n). \tag{4.5}$$

4.1.1 Qubit case

Taking only one qubit, that is, $d = 2$, we are able to solve the model analytically. The initial and final bases $\{|n\rangle\}$ will be the energy eigenbases of $H_i = -h_z/2 \, \sigma_z = -h_z/2 \, |0\rangle\langle 0| + h_z/2 \, |1\rangle\langle 1|$, where $|0\rangle = (1, 0)^\intercal$ and $|1\rangle = (0, 1)^\intercal$ are the eigenvectors of σ_z. First, we write the Hamiltonian H as being proportional to a Pauli matrix of the form $(\boldsymbol{\sigma} \cdot \hat{\boldsymbol{n}}) = \sigma_n = \frac{1}{h}(h_x \sigma_x + h_z \sigma_z)$, where $h = \sqrt{h_x^2 + h_z^2}$ is a normalization constant. Then, the unitary becomes

$$U = \exp\{-iH\tau\} = \exp\left\{ \frac{ih\tau}{2} \sigma_n \right\} = \cos(\theta/2) + i\sigma_n \sin(\theta/2), \tag{4.6}$$

where $\theta = h\tau$ [1]. We proceed by computing the transition probabilities $p_{m|n} = |\langle m|U|n\rangle|^2$. First, we note that

$$\langle m|U|n\rangle = \langle m| \left[\cos(\theta/2) + i\, \frac{\sin(\theta/2)}{h}(h_x \sigma_x + h_z \sigma_z) \right] |n\rangle$$

$$= \delta_{mn} \cos(\theta/2) + i\, \frac{\sin(\theta/2)}{h} \left(h_x \langle m|\sigma_x|n\rangle + h_z \langle m|\sigma_z|n\rangle \right)$$

$$= \begin{cases} \delta_{mn} \left[\cos(\theta/2) \pm i\frac{h_z}{h} \sin(\theta/2) \right], & \text{for } m = n, \\ i\frac{h_x}{h} \sin(\theta/2), & \text{for } m \neq n, \end{cases} \tag{4.7}$$

where $m, n = 0, 1$. Therefore,

$$p_{m|n} = \begin{cases} \delta_{mn} \left[\cos^2(\theta/2) + \frac{h_z^2}{h^2} \sin^2(\theta/2) \right], & \text{for } m = n, \\ \frac{h_x^2}{h^2} \sin^2(\theta/2), & \text{for } m \neq n. \end{cases} \tag{4.8}$$

As a sanity test, we can check some trivial cases. Taking $\tau = 0$, that is, $\theta = 0$, there is no work protocol, as the external parameter is not changed. Indeed, in this case, there is no

---

[1]This result follows from a simple series expansion of $e^{-iH\tau}$, together with the fact that $\sigma_n^2 = 1$

probability of transition from a state $|n\rangle$ to a different state $|m\rangle$, as $\sin^2(\theta/2) \to 0$. Moreover, taking $h_x = 0$, which means $H = H_i = H_f$ and $h = h_z$, also shouldn't change the state of the system. It is truly what happens, as the term for $m \neq n$ goes to zero and the other one goes to 1. Also, summing over m the probabilities for $m = n$ and $m \neq n$ we should have the total probability, and that is the result we obtain.

Returning to the stochastic entropy production, in the case of a qubit, we have only 4 possible transitions: $|0\rangle \to |0\rangle$, $|1\rangle \to |1\rangle$, $|0\rangle \to |1\rangle$, $|1\rangle \to |0\rangle$. From Eq. (4.5), we see that, when the state of the system doesn't change, there is no entropy production. Therefore, $\sigma[0,0] = \sigma[1,1] = 0$. However, when $m \neq n$, we have $\epsilon_0 = \langle 0|H_i|0\rangle = -h_z/2$ and $\epsilon_1 = \langle 1|H_i|1\rangle = h_z/2$, and so

$$\sigma[0,1] = \beta(\epsilon_1 - \epsilon_0) = \beta h_z, \qquad \sigma[1,0] = \beta(\epsilon_0 - \epsilon_1) = -\beta h_z. \tag{4.9}$$

We can also explicitly calculate the populations of the initial thermal state, as it is the final thing we need in order to compute the cumulants of σ. They are given by

$$p_0^i = \frac{e^{-\beta\epsilon_0}}{e^{-\beta\epsilon_0} + e^{-\beta\epsilon_1}} = \frac{1}{1 + e^{-\beta(\epsilon_1 - \epsilon_0)}} = \frac{1}{1 + e^{-\beta h_z}}, \tag{4.10}$$

and

$$p_1^i = \frac{e^{-\beta\epsilon_1}}{e^{-\beta\epsilon_0} + e^{-\beta\epsilon_1}} = \frac{1}{e^{-\beta(\epsilon_0 - \epsilon_1)} + 1} = \frac{1}{e^{\beta h_z} + 1}. \tag{4.11}$$

With the populations (Eqs. (4.10) and (4.11)) and the probabilities (Eq. (4.8)), we obtain the probabilities of a specific trajectory, or else the probabilities of obtaining a certain value of entropy production σ, $P(\sigma) = P[m,n] = p_{m|n}\, p_n^i$. As $\sigma[0,0] = \sigma[1,1] = 0$, we have that $P(0) = P[0,0] + P[1,1] = p_0^i\, p_{0|0} + p_1^i\, p_{1|1}$. The other probabilities are $P(\beta h_z) = p_0^i\, p_{1|0}$ and $P(-\beta h_z) = p_1^i\, p_{0|1}$.

In Figure 4.1, we show how the probabilities depend on each of the parameters of the system (β, τ, h_x and h_z). First, image (a) evidentiates that the probabilities saturate for finite β, and the probability of the entropy being reduced ($P(-\beta h_z)$) goes to zero for large β (small temperature). This entropy production corresponds to the system going from the excited state to the ground state, and it becomes less probable because it becomes less probable for the qubit to start in the excited state at low temperatures (p_1^i in Eq. (4.11) goes to zero as β grows). On the other side, for lower β, or else higher temperature, the probabilities for positive and negative values of the entropy production are equal, as p_0^i and p_1^i (Eqs. (4.10) and (4.11)) become equal.
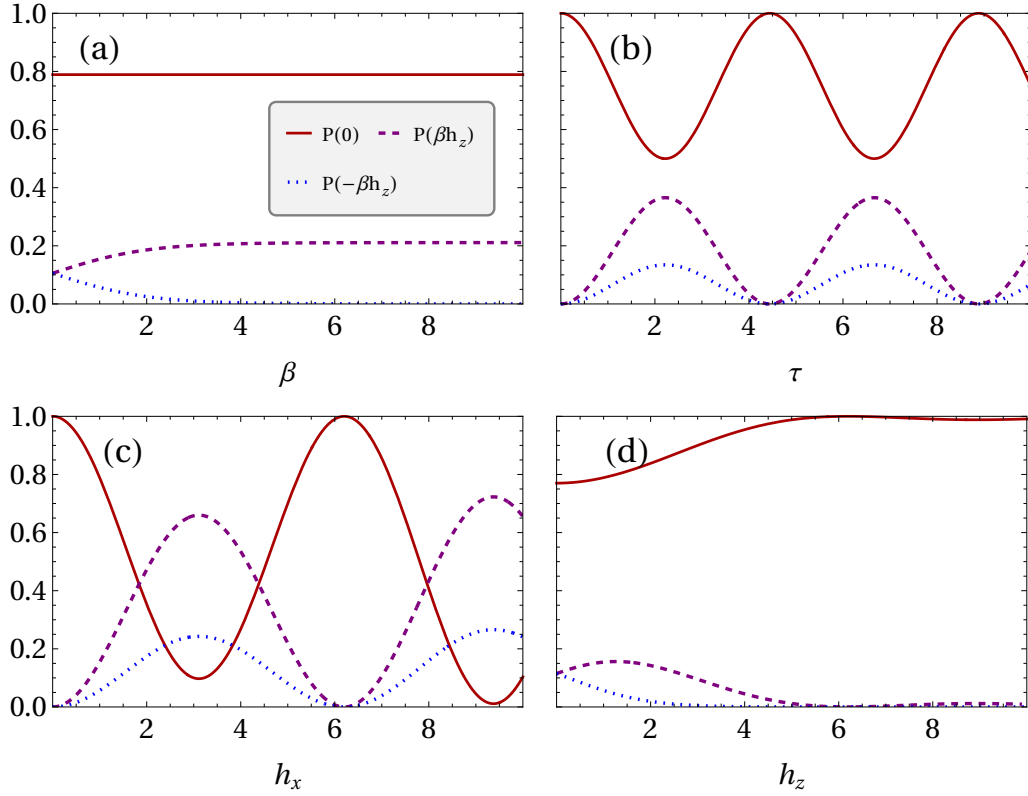
Figure 4.1: Probabilities of the stochastic entropy production for a single qubit (macrospin model) as functions of the different parameters of the system. All values are fixed as $\beta = \tau = h_x = h_z = 1$ for images in which they are not the parameter studied.

From Figures 4.1 (b) and (c), we notice that for certain values of τ and h_x, nothing happens to the qubit and no entropy is produced (when $\theta = h\tau = 2k\pi, k = 0, 1, 2, ...$). Also, from image (c), we notice that there are certain values of h_x for which it is more likely that entropy increases (or decreases) than that nothing happens. Lastly, from image (d), we notice that, as h_z increases in comparison with $h_x = 1$, it becomes more an more probable that no transitions occur and that no entropy is produced.

Now, we proceed with the analytic calculations. With the probabilities (Eqs. (4.8), (4.10) and (4.11)) and the expression for the stochastic entropy production (Eq. (4.9)) in hands, we can compute all its statistical moments. For instance, the average entropy production reads

$$\Sigma = P[0,0]\,\sigma[0,0] + P[1,1]\,\sigma[1,1] + P[0,1]\,\sigma[0,1] + P[1,0]\,\sigma[1,0]$$

$$= p_{1|0}\,p_0^i\,\sigma[0,1] + p_{0|1}\,p_1^i\,\sigma[1,0]$$

$$= \beta h_z \frac{h_x^2}{h^2}\sin^2(\theta/2)\left[\frac{e^{\beta h_z/2}}{e^{\beta h_z/2} + e^{-\beta h_z/2}} - \frac{e^{-\beta h_z/2}}{e^{\beta h_z/2} + e^{-\beta h_z/2}}\right]$$

$$= \beta h_z \frac{h_x^2}{h^2}\sin^2(\theta/2)\tanh(\beta h_z/2), \tag{4.12}$$

where, again, $\theta = h\tau$. As a sanity check, we note that $\Sigma \geq 0$, since it is an even function of both h_x and h_z. It is also interesting to look at the variance of σ, $\mathrm{Var}(\sigma) = \langle \sigma^2 \rangle - \langle \sigma \rangle^2$. First, we have that

$$
\begin{aligned}
\langle \sigma^2 \rangle &= \sum_{n,m} P[n,m]\sigma[n,m]^2 \\
&= p_{1|0}\, p_0^i\, \sigma[0,1]^2 + p_{0|1}\, p_1^i\, \sigma[1,0]^2 \\
&= \beta^2 h_z^2 \frac{h_x^2}{h^2} \sin^2(\theta/2) \sum_n p_n^i \\
&= \beta^2 h_z^2 \frac{h_x^2}{h^2} \sin^2(\theta/2).
\end{aligned}
\tag{4.13}
$$

The second term is just the average squared, so the variance is given by

$$
\mathrm{Var}(\sigma) = \beta^2 h_z^2 \frac{h_x^2}{h^2} \sin^2(\theta/2) \left[1 - \frac{h_x^2}{h^2} \sin^2(\theta/2) \tanh^2(\beta h_z/2) \right].
\tag{4.14}
$$

As expected, the variance is also positive, because both $\sin^2(\theta/2)$ and $\tanh^2(\beta h_z/2)$ are always between 0 and 1, and h_x^2/h^2 is always smaller than 1.

For higher dimensions, however, it is not possible to develop the calculations analytically. Therefore, we proceed with a numerical analysis for arbitrary dimension.

4.1.2 Numerical analysis for arbitrary dimension

In order to analyse how the probability distribution of the stochastic entropy production behaves considering the model of the macrospin proposed, we solved it numerically. For simplicity, we set $h_z = 1$ for all the simulations, and observed how the distributions changed with respect to the dimension d of the Hilbert space, the inverse temperature β, the time of evolution τ and the magnitude of the pulse in the x-direction h_x.

First, we focus on the dependence with the dimension of the system. In Figure 4.2 we show the probability distributions of the stochastic entropy production for different values of d. Considering the macrospin model, when $d \to \infty$ (thermodynamic limit), we would expect the system to behave as a classical microscopical spin . For larger values of d, we notice that the probability distributions start to indicate Gaussian behavior. In images (d) and (e), we superimpose a plot of the Gaussian distributions that have the same average and standard deviation as the corresponding probability distributions. The curve fits the data, which indicates that indeed the

entropy production fluctuations become asymptotically Gaussian in the thermodynamic limit.

Figure 4.2: Probability distributions of the stochastic entropy production σ for different values of d for the macrospin model. Other parameters are fixed: $\beta = 10$, $\tau = 1$ and $h_x = 0.5$. Images (a) through (e) have $d = 10, 20, 50, 100$ and 200, respectively. In (d) and (e), the dashed gray curve represents a Gaussian with same average and standard deviation as the corresponding probability distributions.
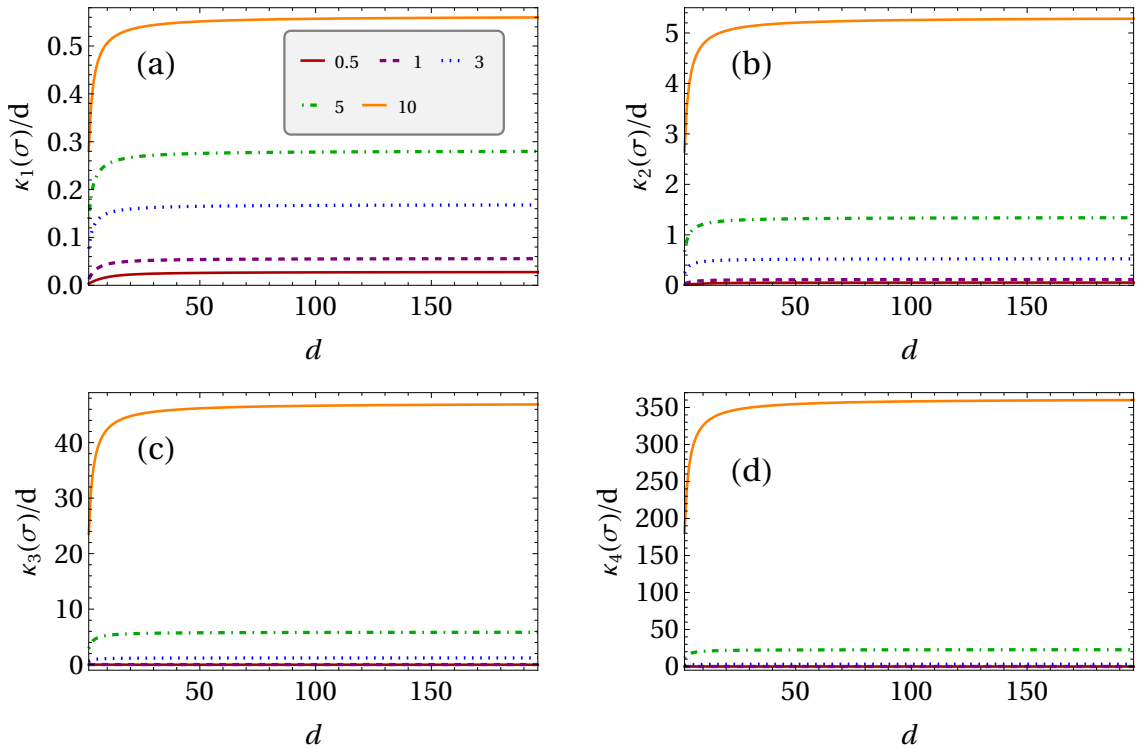
Figure 4.3: Cumulants of the entropy production as a function of the dimension d for the macrospin model. The plots show different values of β and are scaled by d. Other parameters are fixed: $\tau = 1$ and $h_x = 0.5$.

To further analyse the dependence on the dimension, we show in Figure 4.3 the first four cumulants of the distribution of the entropy production as functions of d. We notice that, for d large enough, eventually all the cumulants start to scale linearly with the dimension. The

concept of "large enough", however, varies according to the inverse temperature β. For example, considering the fourth cumulant $\kappa_4(\sigma)$ on image (d), for $\beta = 0.5$, the dependence with d starts to become approximately linear for $d > 150$, while for the other values of β, for $d > 30$ that is already the case. This indicates that the dimension for which the system starts having a Gaussian behavior depends on the temperature.
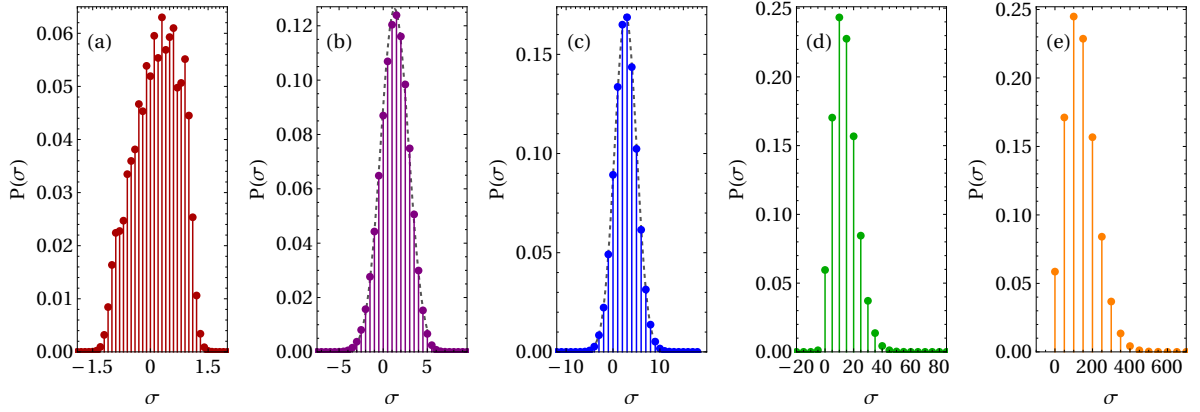
Figure 4.4: Probability distributions of the stochastic entropy production σ for different values of β for the macrospin model. Plots (a) through (c) have $\beta = 0.1, 0.5, 1, 5$ and 50, respectively. Other parameters are fixed: $d = 50$, $\tau = 1$ and $h_x = 0.5$.

The dependence on β can be seen in Figure 4.4, for fixed $d = 50$. The distributions for $\beta = 0.5$ and $\beta = 1$ seem to be Gaussian, but those for $\beta = 0.1$, $\beta = 5$ and $\beta = 50$ do not. However, despite the value of β, there seems to always be a sufficiently large value of d for which the probability distribution tends to a Gaussian. The plots for $\beta = 0.1$ and $\beta = 100$ are shown in Figures 4.5 and 4.6.
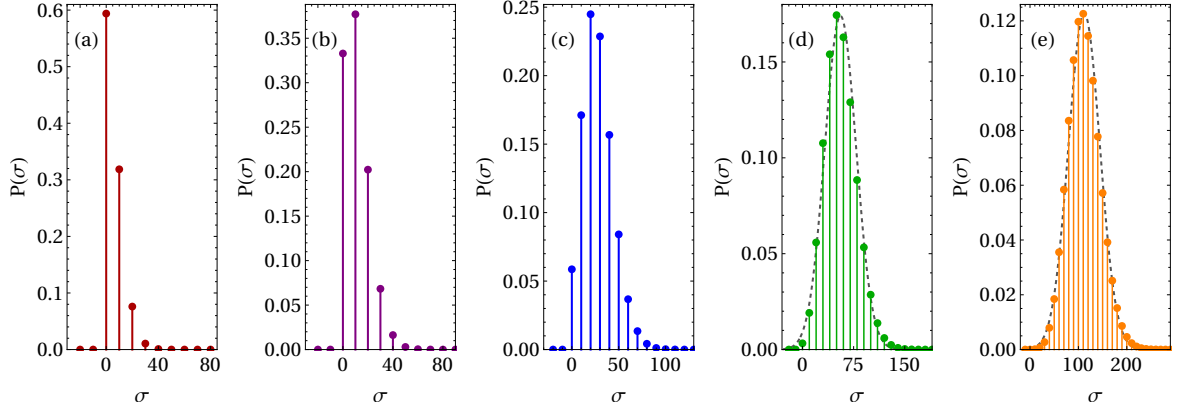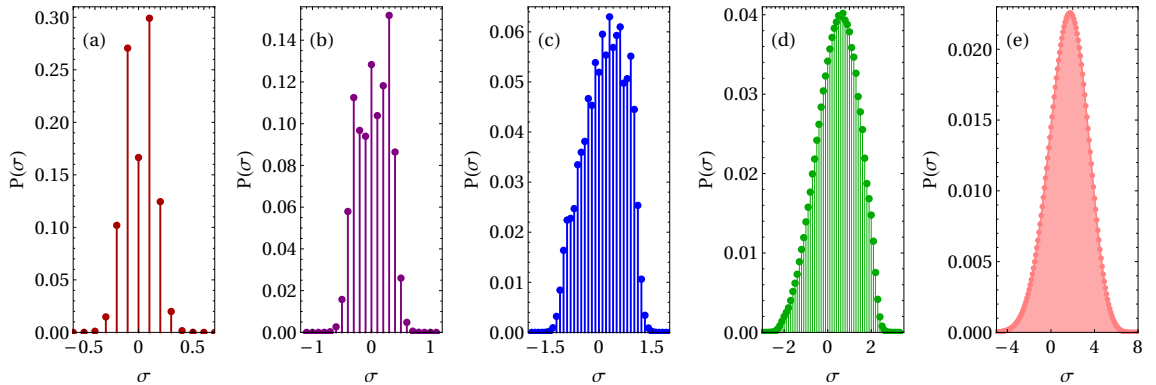

Figure 4.5: Probability distributions of the stochastic entropy production σ for different values of d for the macrospin model. Plots (a) through (e) have $d = 10, 20, 50, 100$ and 300, respectively. Other parameters are fixed: $\beta = 0.1$, $\tau = 1$ and $h_x = 0.5$.

Figure 4.7 shows the first four cumulants, now as a function of β for different values of d. As can be seen, the cumulant κ_n is scaled by β^n. This therefore serves as evidence that, at low
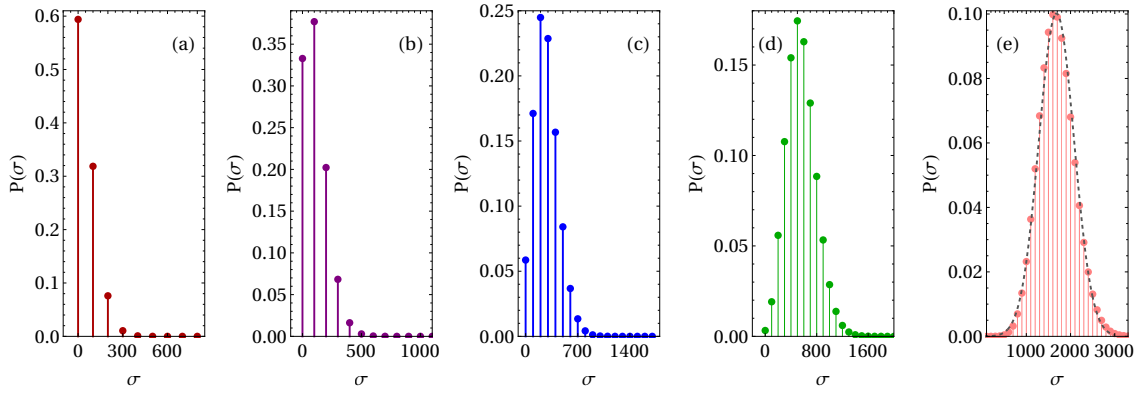
Figure 4.6: Same as Figure 4.5 but for $\beta = 100$.

temperatures, all cumulants scale with simple powers of β. We also notice, from Fig. 4.4, that for lower β, the support is larger. That is due to the fact that, for higher temperatures, there is a higher number of transitions that may happen.
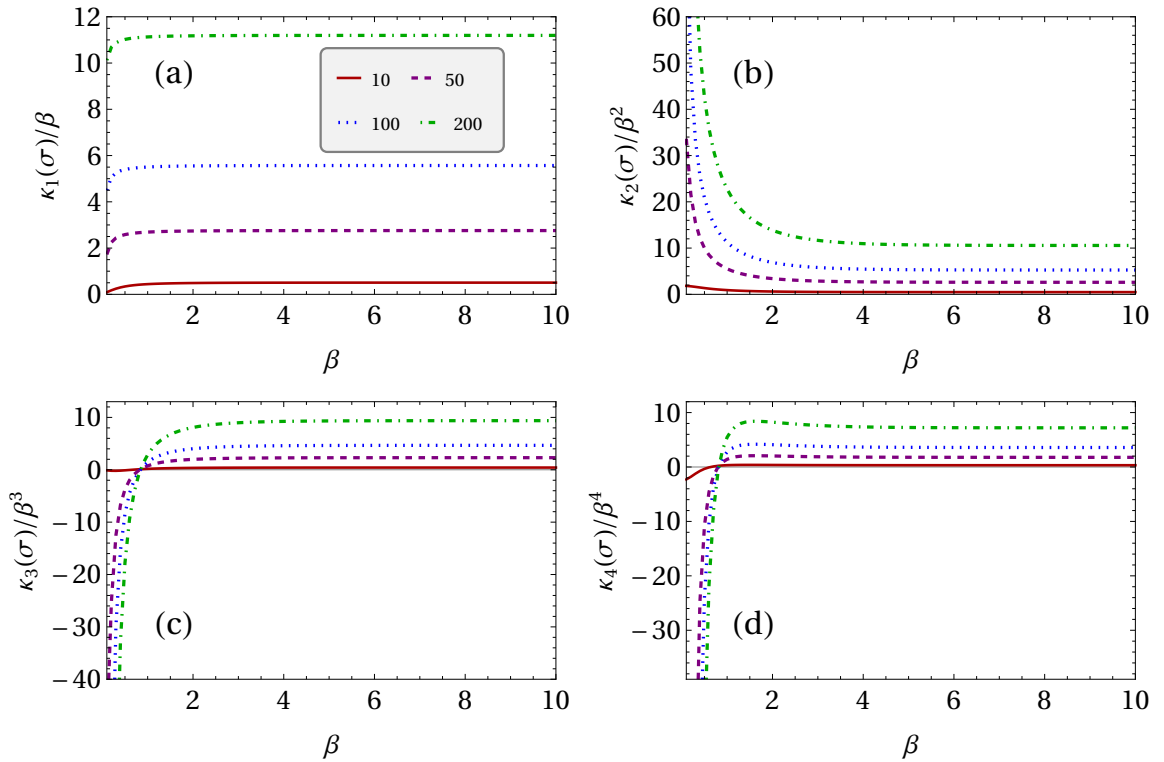
Figure 4.7: Cumulants of the entropy production as a function of β for different values of d (macrospin model). Other parameters are fixed: $\tau = 1$ and $h_x = 0.5$.

Differently than d and β, the dependence of the probabilities and cumulants with τ and h_x is not simple. Plots as functions of both parameters are shown in Figures 4.8 and 4.9. We see that the cumulants are generally oscillatory in τ and h_x.
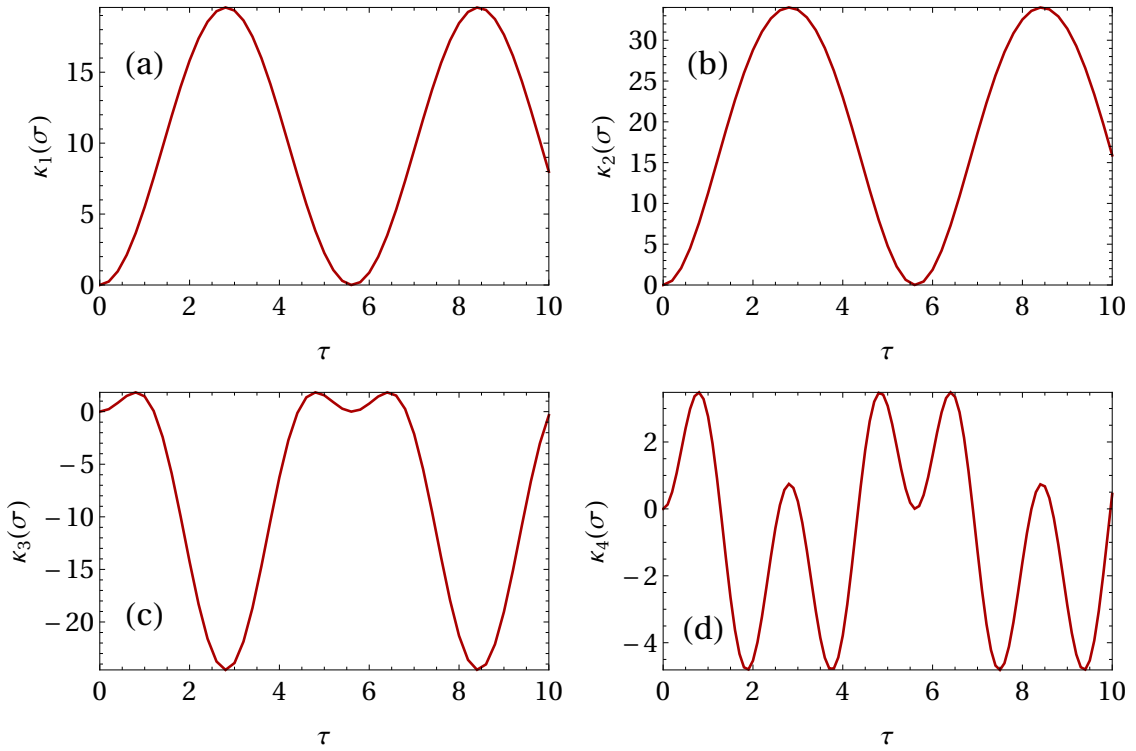
Figure 4.8: Cumulants of the entropy production as a function of τ for the macrospin model. Other parameters are fixed: $d = 100$, $\beta = 1$ and $h_x = 0.5$.
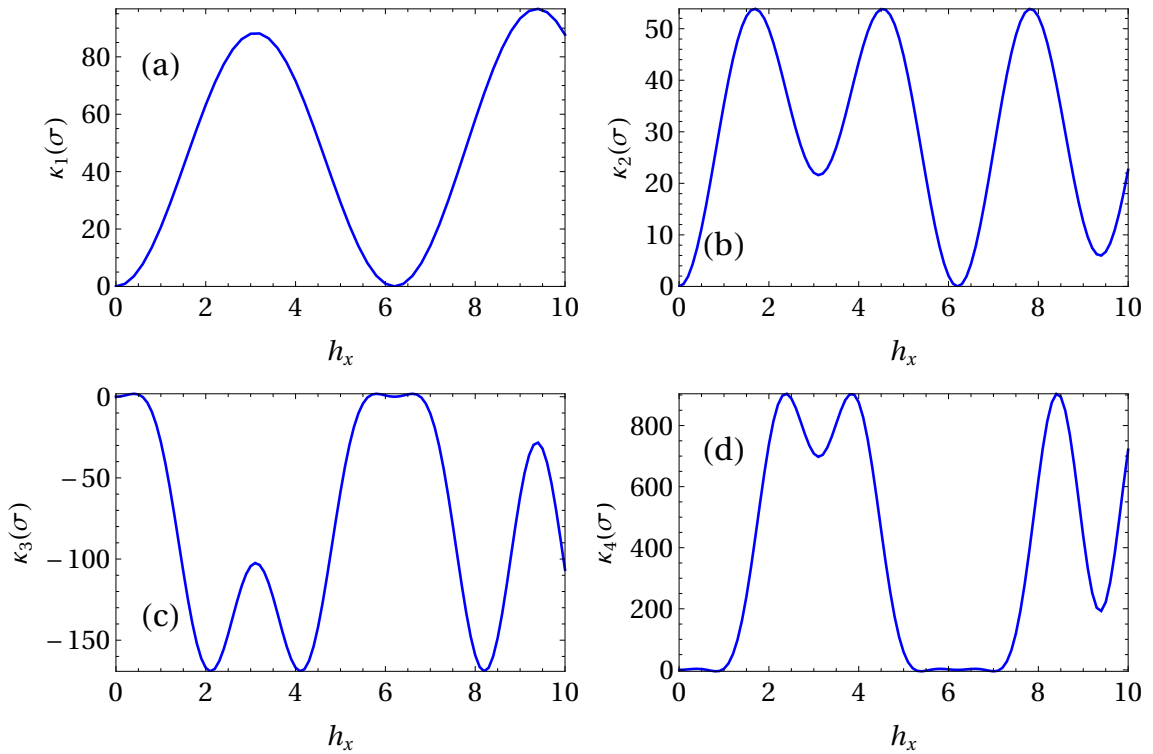
Figure 4.9: Cumulants of the entropy production as a function of h_x for the macrospin model. Other parameters are fixed: $d = 100$, $\beta = 1$ and $\tau = 1$.

4.2 LMG model

The Lipkin-Meshkov-Glick (LMG) model [7–9] , besides its similarities with the macrospin model, presents a phase transition on the ground state energy of the Hamiltonian. It has been shown that this phase transition affects the entropy production in a non-trivial way [57].

The model represents a system of dimension $d = 2S + 1$ that is fully connected and can be collective described by a macrospin, as the one previously presented in Sec. 4.1. Its Hamiltonian is given by

$$H = -\frac{J}{2s}S_x^2 - gS_z,$$
(4.15)

where $J > 0$ is the coupling constant between the spins, $g > 0$ is the transverse field and s is the total spin. Before we present the work protocol that follows from this Hamiltonian, we first expose how the phase transition emerges.

4.2.1 Phase transition in the thermodynamic limit

The Hamiltonian of the LMG model is not diagonal and it is not trivial to encounter its eigenvalues and eigenvectors for any dimension. However, when we consider the thermodynamic limit (i.e., $S \to \infty$), the diagonalization can be done in two steps [58]: we first solve for the classical ground state and then add the quantum fluctuations. For the scope of this work, we will only focus on the classical ground state, as we are only interested, at this moment, in identifying the phase transition and not on the energy eigenstates themselves. Afterwards, we will deal with the problem numerically for arbitrary dimension.

First, it is necessary to define the so-called spin-coherent state [57,59],

$$|\Omega\rangle = e^{-i\phi S_z}e^{-i\theta S_y}|s\rangle,$$
(4.16)

where $\theta \in [0, \pi]$ and $\phi \in [0, 2\pi)$ are polar coordinates and $|S\rangle$ is the eigenvector of S_z with eigenvalue S. This state is the closest quantum analog to a classical spin state, and it allows us to write the projections of the spin onto the x, y and z axes as [57]

$$(\langle S_x\rangle, \langle S_y\rangle, \langle S_z\rangle) = S(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta).$$
(4.17)

Also, it has been shown [59] that, in the thermodynamic limit, the leading order of the ground state of H is given by the spin-coherent state $|\Omega\rangle$. Therefore, the energy of the ground state

is given by the angles θ, ϕ minimizing the function $E(\theta, \phi) = \langle \Omega | H | \Omega \rangle$. In the limit where $S \to \infty$, we can approximate $\langle S_x^2 \rangle \approx \langle S_x \rangle^2$, and so the energy E is given by

$$E(\theta, \phi) = -s \left(\frac{J}{2} \sin^2 \theta \cos^2 \phi + g \cos \theta \right). \tag{4.18}$$

Our objective is to minimize the energy with respect to the polar coordinates θ and ϕ, so it is necessary that the derivatives with respect to these parameters are equal to zero, that is,

$$\frac{\partial E}{\partial \theta} = s \left(-J \sin \theta \cos \theta \cos^2 \phi + g \sin \theta \right) = 0, \tag{4.19}$$

$$\frac{\partial E}{\partial \phi} = s \, J \sin^2 \theta \cos \phi \sin \phi = 0. \tag{4.20}$$

The first solution is $\sin \theta = 0$, i.e., $\theta = 0$ ($\theta = \pi$ is a possible formal solution, but inserting it back into the expression for the energy shows that it is a maximum of the function, not a minimum as desired). This solution imposes no condition over the other parameters (ϕ). Besides that, we have two other possibilities: $\cos \phi = 0$ or $\sin \phi = 0$. The first one is only possible if $g = 0$, which is not what we want. The second one, $\sin \phi = 0$, however, imposes a condition over the other parameters that results in the phase transition. It requires that $\phi = 0$ or $\phi = \pi$, which leads to $\cos^2 \phi = 1$, and implies that we must have $\cos \theta = g/J$. This solution only exists for $g < J$ (as $\cos \theta \in [0, 1]$).

In summary, for $g > J$, there is only one possible solution: $\theta = 0$, with no restriction to ϕ. However, when $g < J$, two other solutions emerge: $\phi = 0$ or $\phi = \pi$. This motivates the definition of the magnetization in the $m = \sin \theta \cos \phi$, which takes place as the order parameter of the phase transition; for $g > J$, it is identically zero, and otherwise it is given by [57]

$$m = \pm \sin \theta = \pm \sqrt{g_c^2 - g^2}/J. \tag{4.21}$$

A plot of the magnetization as a function of g can be seen in Figure 4.10.

A physical interpretation can be given to the phase transition and the magnetization. First, we notice that $m = \langle S_x \rangle / S$, that is, the magnetization is proportional to the projection of the spin into the x-axis. For $g > J$, the external field aligned with the z-direction wins the competition against the internal forces J of the collective spin: $\theta = 0$, which means that the spin has no projection onto the x- and y-axes, and therefore the magnetization is zero [58].
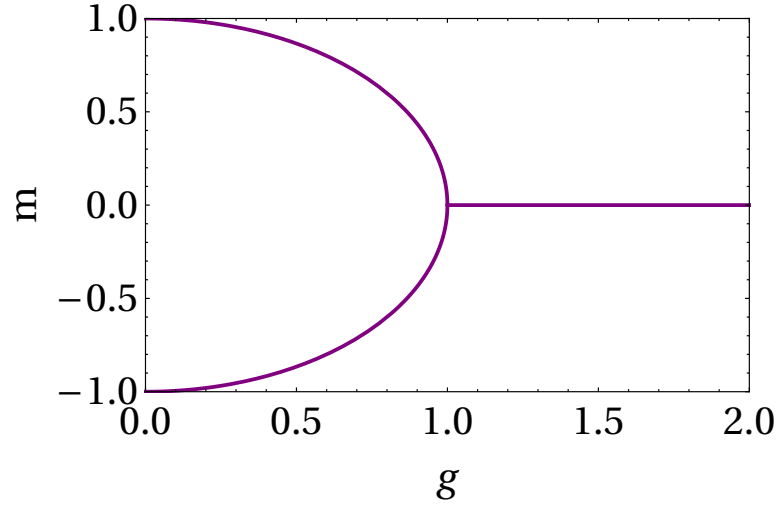
Figure 4.10: Magnetization m, given in Eq. (4.21), as a function of the transverse magnetic field g. The other parameters are set as $g_c = J = 1$.

However, in the case where $g < J$, the system behaves as a ferromagnetic material. If $g = 0$, the spin is aligned with the x-axis, either up or down. When there is a field applied, the spin starts to tilt to the z-direction according to the ratio between the external field strength and the internal forces of the system.

4.2.2 Work protocol on LMG model

Now that we understood how the phase transition emerges on the LMG model, we will see how it affects the entropy production at the stochastic level. In this case, we will consider that a collective spin system is subject to the LMG Hamiltonian $H = -J/(2s)S_x^2 - g(t)S_z$, such that the transverse field intensity $g(t)$ changes with time. For simplicity, in our protocol, we will consider that g is changed by means of a quench: it instantaneously changes from g_i to $g_f = g_i + \delta g$, where $\delta g \ll g_i$.

Again we consider that the system begins in the thermal state of the initial Hamiltonian $H_i = -J/(2s)S_x^2 - g_i S_z = \sum_{n=0}^{d-1} \epsilon_n^i |n\rangle\langle n|$ (where the eigenvalues and eigenvectors are now computed numerically). That is

$$\rho_i^{th} = \frac{e^{-\beta H_i}}{Z_i} = \sum_n p_n^i |n\rangle\langle n|, \tag{4.22}$$

where, again, $p_n^i = e^{-\beta \epsilon_n}/Z_i$, $Z_i = \text{tr}\{e^{-\beta H_i}\}$ is the partition function. The measurement on the eigenbasis of H_i results in outcome $|n\rangle$ with probability p_n^i. Then, the external field is abruptly changed to g_f, which means that $\tau \to 0$, $U \to 1$, and therefore $\rho_\tau = U\rho_i^{th}U^\dagger = \rho_i^{th}$. At

the end, the system is measured in the basis of the final Hamiltonian $H_f = -J/(2s)S_x^2 - g_f S_z = \sum_{m'=0}^{d-1} \epsilon_{m'}^f |m'\rangle\langle m'|$, resulting in $|m'\rangle$ with probability $p_{m'}^\tau = \langle m'|\rho_i^{th}|m'\rangle$.

In Section 3.2.4 we have shown the general expression for the stochastic entropy production in the case of quenches with infinitesimal changes to the Hamiltonian. However, it depends on the eigenvectors and eigenvalues of the initial Hamiltonian and, as we have said, they are not easy to compute for arbitrary dimensions. Therefore, we will show some numerical results for the statistics of the entropy production in the LMG model.

4.2.3 Numerical results

The probability distributions for different dimensions are depicted in Figure 4.11. Differently than what we would expect considering the results obtained for the macrospin (Fig. 4.2), we notice that the distributions do not seem to tend to a Gaussian. We chose the parameters so that we have a large number of transitions ($g = 0.9$ and β small), but even for dimensions as high as $d = 3000$ we do not see the same behavior as for the macrospin.
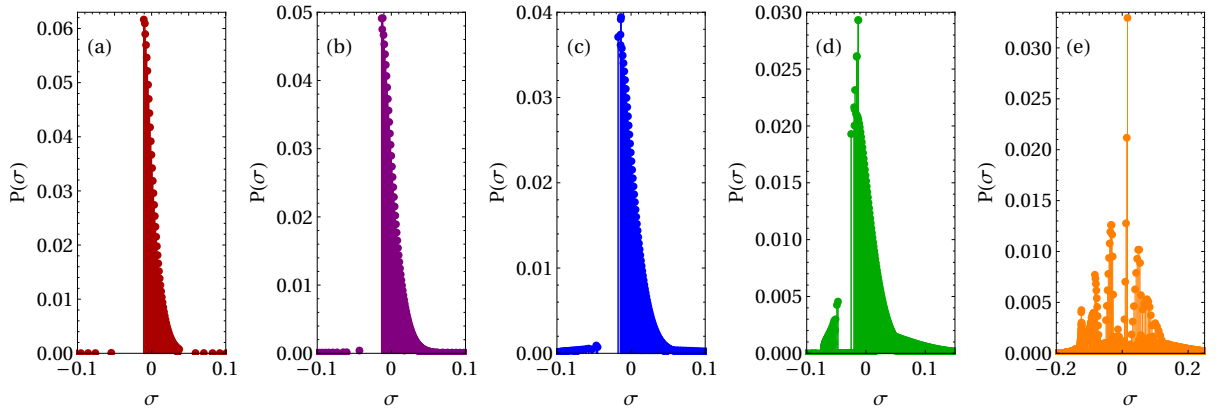
Figure 4.11: Probability distributions of the stochastic entropy production σ for different values of d for the LMG model. Other parameters are fixed: $\beta = 0.1$, $g = 0.9$ and $\delta g = 0.01$. Images (a) through (e) have $d = 50, 100, 200, 500$ and 3000, respectively.

In Figures 4.12 and 4.13 we show the dependence of the cumulants with the magnitude of the transverse field g. As expected, the phase transition in $g = 1$ is observed in all the cumulants for higher dimensions. Another interesting aspect to notice is that, even though the probability distributions do not look alike, the dependence of the cumulants with d and β is similar to that of the macrospin model; all of them depend linearly on the dimension and scale with β^n, where n is the order of the cumulant.
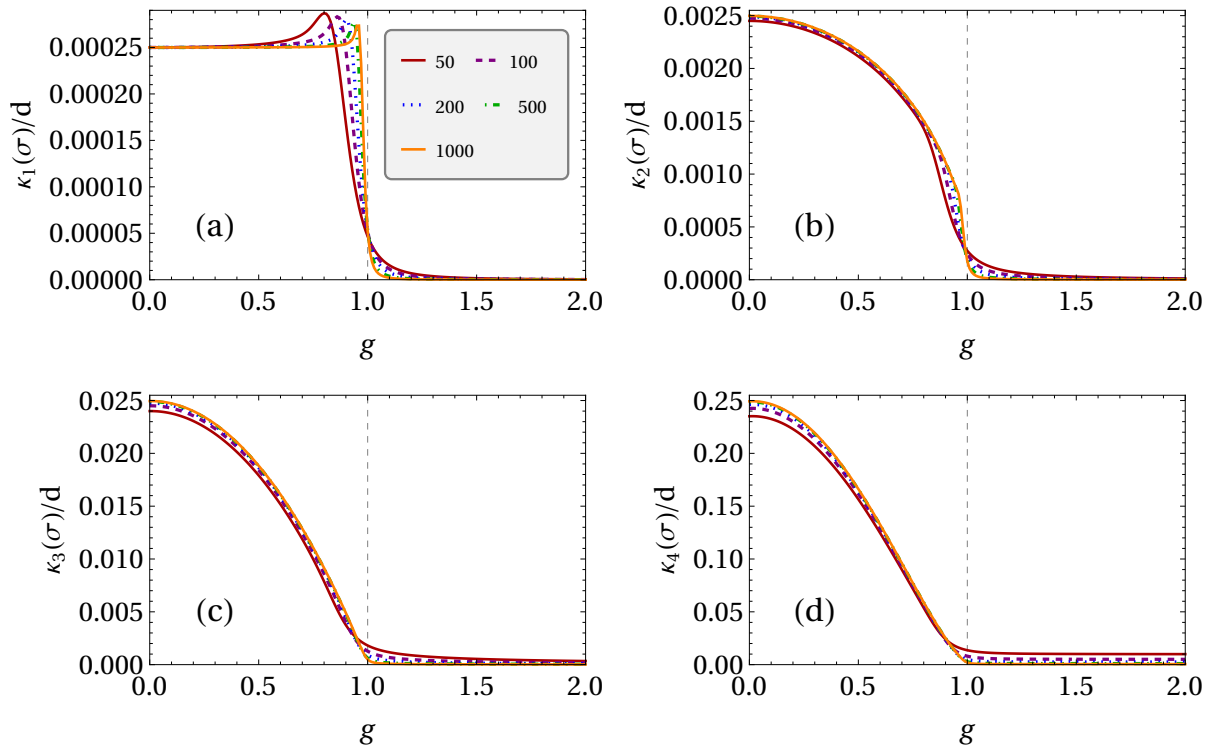
Figure 4.12: Cumulants of the entropy production as a function of g for the LMG model. The plots show different values of d and are scaled by d. Other parameters are fixed: $\beta = 10$ and $\delta g = 0.01$.
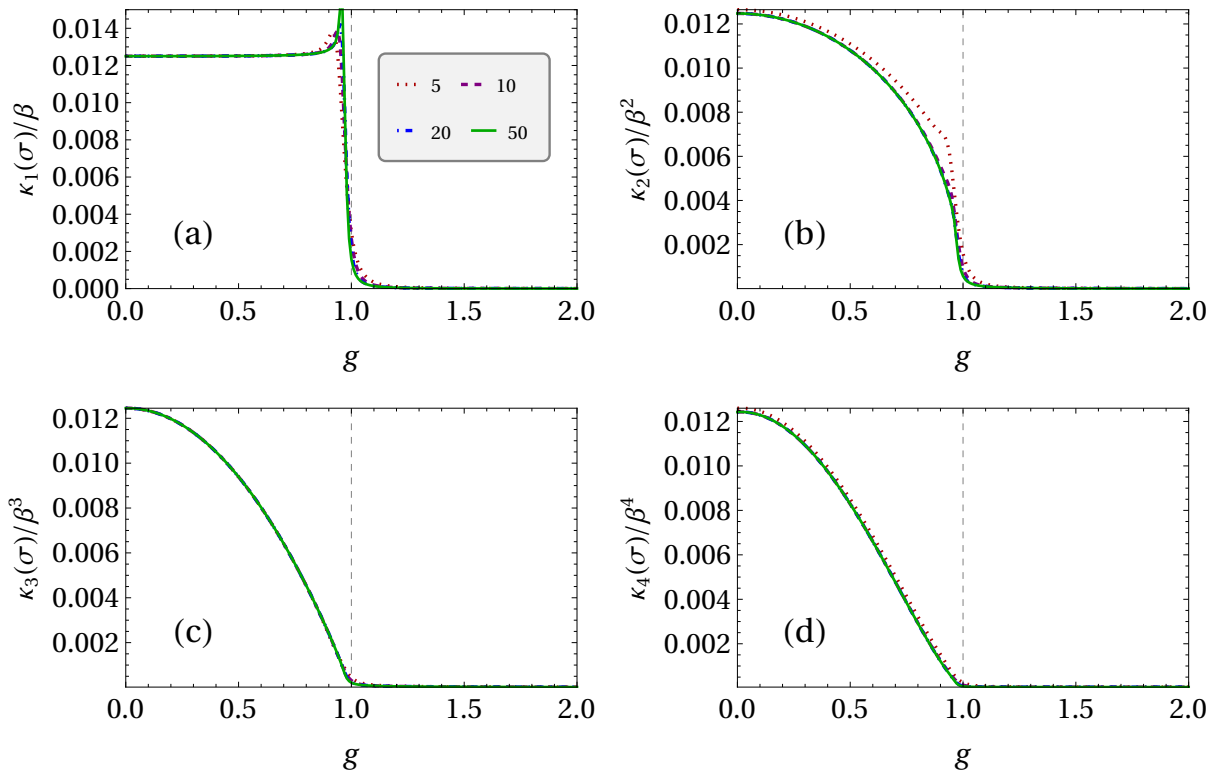
Figure 4.13: Cumulants of the entropy production as a function of g for the LMG model. The plots show different values of β and are scaled by powers of β. Other parameters are fixed: $d = 500$ and $\delta g = 0.01$.

Chapter 5

Coherent contribution to entropy production: Γ splitting

Entropy production in work protocols is related to an entropic distance between the state obtained by unitary evolution and the final thermal state. This entropic distance comes from two different contributions: one from changes in coherences and the other from populations. Those could also be classified as quantum and classical contributions, as coherence is a purely quantum resource.

Our intention is to understand how the quantum part of entropy production behaves stochastically. However, there is no unique way of identifying which part of the entropy production comes from changes in non-diagonal terms. In this chapter, we will study the splitting proposed in References [2, 3]. It states that the coherent contributions come from the difference in entropy between the final state and the dephased state in the basis of the final Hamiltonian (defined in Eq. (5.1) below). In comparison, in Chapter 6 we will present another splitting, that considers, instead of the dephased final state, the dephased Hamiltonian as the source of coherent contributions.

First, recall the work protocol exposed in Sec. 3.2.2: a system, initially in the thermal state $\rho_i^{th} = e^{-\beta H_i}/Z_i$ is driven by the external Hamiltonian H to state ρ_τ. The total entropy production is given by $\Sigma = S(\rho_\tau || \rho_f^{th})$, where $\rho_f^{th} = e^{-\beta H_f}/Z_f$. The final state ρ_τ dephased with respect to the energy basis of H_f, taking $H_f = \sum_{m'} \epsilon_{m'}^f |m'\rangle\langle m'|$, is defined as

$$\Delta_f[\rho_\tau] := \sum_{m'} |m'\rangle\langle m'| \, \rho_\tau \, |m'\rangle\langle m'| \,. \tag{5.1}$$

Now, by adding and subtracting the entropy of $\Delta_f[\rho_\tau]$ to the expression for the entropy production, we get

$$
\begin{aligned}
\Sigma &= S(\Delta_f[\rho_\tau]) - S(\Delta_f[\rho_\tau]) - S(\rho_\tau) - \mathrm{tr}\big(\rho_\tau \log \rho_f^{th}\big) \\
&= \mathcal{C}(\rho_\tau) + \mathrm{tr}\big[\Delta_f[\rho_\tau] \log \Delta_f[\rho_\tau] - \rho_\tau \log \rho_f^{th}\big] \\
&= \mathcal{C}(\rho_\tau) + \mathrm{tr}\big[\Delta_f[\rho_\tau] \log \Delta_f[\rho_\tau] - \Delta_f[\rho_\tau] \log \rho_f^{th}\big] \\
&= \mathcal{C}(\rho_\tau) + S(\Delta_f[\rho_\tau] || \rho_f^{th}),
\end{aligned}
\tag{5.2}
$$

where $\mathcal{C}(\rho_\tau) = S(\Delta_f[\rho_\tau]) - S(\rho_\tau)$ is the relative entropy of coherence, as defined in Eq. 2.27, and we have used the fact that $\mathrm{tr}\big(\rho_\tau \log \rho_f^{th}\big) = \mathrm{tr}\big(\Delta_f[\rho_\tau] \log \rho_f^{th}\big)$. We identify the first term as the contribution from coherences, as it compares the actual final state with its diagonal version. The second contribution encompasses the differences in populations between the final state and the desired thermal state, and therefore we associate it with the classical contribution. We will follow the notation from Reference [5] and denote the terms as

$$
\Gamma_{\mathrm{qu}} := \mathcal{C}(\rho_\tau),
\tag{5.3}
$$

$$
\Gamma_{\mathrm{cl}} := S(\Delta_f[\rho_\tau] || \rho_f^{th}).
\tag{5.4}
$$

It is simple to notice that $\Gamma_{\mathrm{cl}} \geq 0$, as the relative entropy is always non-negative. As for Γ_{qu}, we can rewrite it as a relative entropy as well, that is,

$$
\begin{aligned}
\Gamma_{\mathrm{qu}} &= S(\Delta_f[\rho_\tau]) - S(\rho_\tau) \\
&= \mathrm{tr}(\rho_\tau \log \rho_\tau) - \mathrm{tr}(\Delta_f[\rho_\tau] \log \Delta_f[\rho_\tau]) \\
&= \mathrm{tr}(\rho_\tau \log \rho_\tau) - \mathrm{tr}(\rho_\tau \log \Delta_f[\rho_\tau]) \\
&= S(\rho_\tau || \Delta_f[\rho_\tau]) \geq 0.
\end{aligned}
\tag{5.5}
$$

Throughout this chapter, we will focus mainly on Γ_{qu}, but first let us analyse how both of them behave stochastically.

5.1   Stochastic trajectories

We will consider the same work protocol proposed in Sec. 3.2.2 and the quantum trajectory from the two-point measurement (TPM) scheme. Considering $H_i = \sum_n \epsilon_n^i |n\rangle\langle n|$ and $H_f = \sum_{m'} \epsilon_{m'}^f |m'\rangle\langle m'|$, the probability that the first measurement results in state $|n\rangle$ and the second measurement, performed after the unitary evolution, results in state $|m'\rangle$, is given by

$$P[n, m'] = p_{m'|n}\, p_n^i = |\langle m'|U|n\rangle|^2\, p_n^i. \tag{5.6}$$

We already know that the stochastic total entropy production $\sigma[n, m']$ is given by Eq. 3.20. As for the quantum and classical part, as shown in Reference [2], they are defined as

$$\gamma_{\text{qu}}[n, m'] = \log p_n^i - \log p_{m'}^\tau, \tag{5.7}$$

$$\gamma_{\text{cl}}[n, m'] = \log p_{m'}^\tau - \log p_{m'}^f, \tag{5.8}$$

where $p_{m'}^\tau = \langle m'|\rho_\tau|m'\rangle$. It is easy to see that, if we sum both quantities, it results in $\sigma[n, m'] = \log p_n^i - \log p_{m'}^f$, as expected. We can also check that their averages indeed correspond to Eqs. (5.3) and (5.4). Again considering that $\sum_{m'} p_{m'|n} = 1$ and $\sum_n p_{m'|n}\, p_n^i = p_{m'}^\tau$ (already proven in Sec. 3.2.3), we have

$$
\begin{aligned}
\langle \gamma_{\text{qu}}[n, m'] \rangle &= \sum_{n,m'} \gamma_{\text{qu}}[n, m'] P[n, m'] \\
&= \sum_{n,m'} p_{m'|n}\, p_n^i \log p_n^i - \sum_{n,m'} p_{m'|n}\, p_n^i \log p_{m'}^\tau \\
&= \sum_n p_n^i \log p_n^i - \sum_{m'} p_{m'}^\tau \log p_{m'}^\tau \\
&= -S(\rho_i^{th}) + S(\Delta_f[\rho_\tau]) \\
&= \Gamma_{\text{qu}},
\end{aligned}
\tag{5.9}
$$

as $S(\rho_i^{th}) = S(\rho_\tau)$, given that the evolution is unitary. Doing the same for $\gamma_{cl}[n, m']$,

$$
\begin{aligned}
\langle \gamma_{cl}[n, m'] \rangle &= \sum_{n,m'} \gamma_{cl}[n, m'] P[n, m'] \\
&= \sum_{n,m'} p_{m'|n}\, p_n^i \left(\log p_{m'}^\tau - \log p_{m'}^f \right) \\
&= \sum_{m'} p_{m'}^\tau \left(\log p_{m'}^\tau - \log p_{m'}^f \right) \\
&= S(\Delta_f[\rho_\tau] || \rho_f^{th}) \\
&= \Gamma_{cl}.
\end{aligned}
\tag{5.10}
$$

Such as the stochastic entropy production, we can see that γ_{qu} and γ_{cl} have their own Jarzynski's equalities [52], as stated in Reference [2]; that is, we can write $\langle e^{-\gamma_{qu}} \rangle = \langle e^{-\gamma_{cl}} \rangle = 1$. The proof is given in Appendix B.

From now on, as we are interested in the contribution that stems from coherences, we will focus on the statistics of $\gamma_{qu}[n, m']$. The expression for the variance and other cumulants of γ_{qu} are shown in Appendix C.

5.2 Limiting cases for stochastic coherence in work protocols

We follow the analysis by revisiting the limiting cases proposed in Sec. 3.2.4, one for a quick quench and cyclic process and the other for an instantaneous quench with an infinitesimal perturbation.

5.2.1 $H_f = H_i$ and small τ

In this case, we recall that the unitary can be expanded until order τ^2, resulting in $U = \exp\{-iH\tau\} \approx 1 - iH\tau - H^2\tau^2/2$. Also, the final basis is equal to the initial one, $|n\rangle$. We obtained previously that the trajectory probability $P[n, m]$ was given by (Eq. (3.34))

$$
P[n, m] = \delta_{mn}\, p_n^i + \tau^2\, p_n^i \big(|\langle m|H|n\rangle|^2 - \delta_{mn}\langle n|H^2|n\rangle \big).
\tag{5.11}
$$

To calculate $\gamma_{\text{qu}}[n, m] = \log p_n^i - \log p_m^\tau$, we still have to obtain p_m^τ. It is given by

$$
\begin{aligned}
p_m^\tau &= \langle m| U \rho_i^{th} U^\dagger |m\rangle \\
&\approx \langle m| \left(1 - iH\tau - \frac{H^2\tau^2}{2}\right) \rho_i^{th} \left(1 + iH\tau - \frac{H^2\tau^2}{2}\right) |m\rangle \\
&= \langle m| \rho_i^{th} |m\rangle - i\tau\left(\langle m| H\rho_i^{th} |m\rangle - \langle m| \rho_i^{th} H |m\rangle\right) \\
&\quad - \frac{\tau^2}{2}\left(\langle m| H^2\rho_i^{th} |m\rangle + \langle m| \rho_i^{th} H^2 |m\rangle - 2\langle m| H\rho_i^{th} H |m\rangle\right) + \mathcal{O}(\tau^3) \\
&= \langle m| \rho_i^{th} |m\rangle - i\tau \langle m| \left[H, \rho_i^{th}\right] |m\rangle - \frac{\tau^2}{2} \langle m| [H, [H, \rho_i^{th}]] |m\rangle + \mathcal{O}(\tau^3). \quad (5.12)
\end{aligned}
$$

Analyzing term by term, we find that the linear term in τ will result in

$$
\begin{aligned}
\langle m| H\rho_i^{th} |m\rangle &= \sum_n \langle m| Hp_n^i |n\rangle \langle n|m\rangle = p_m^i \langle m|H|m\rangle \\
&= \langle m| \rho_i^{th} H |m\rangle, \quad (5.13)
\end{aligned}
$$

from which we obtain

$$
\langle m| \left[H, \rho_i^{th}\right] |m\rangle = 0. \quad (5.14)
$$

By simplifying the term proportional to τ^2 in a similar manner, we obtain

$$
\langle m| \left[H, \left[H, \rho_i^{th}\right]\right] |m\rangle = 2\, p_m^i \langle m|H^2|m\rangle - 2 \langle m|H\rho_i^{th} H|m\rangle. \quad (5.15)
$$

Finally, we get

$$
p_m^\tau = p_m^i + \tau^2 \Delta m, \quad (5.16)
$$

where

$$
\Delta m = \langle m|H\rho_i^{th} H|m\rangle - p_m^i \langle m|H^2|m\rangle. \quad (5.17)
$$

Therefore, $\gamma_{\text{qu}}[n, m]$ is given by

$$
\begin{aligned}
\gamma_{\text{qu}}[n, m] &= \log p_n^i - \log p_m^\tau = \log p_n^i - \log\{p_m^i + \tau^2 \Delta m\} \\
&= \log p_n^i - \log\{p_m^i(1 + \tau^2 \Delta m/p_m^i)\} \\
&= \log p_n^i - \log p_m^i - \log\left(1 + \tau^2 \Delta m/p_m^i\right). \quad (5.18)
\end{aligned}
$$

Using the fact that $\log(1 + x) \approx x, x \ll 1$, we finally arrive at

$$\gamma_{\text{qu}}[n, m] = \log p_n^i / p_m^i - \tau^2 \frac{\Delta m}{p_m^i}, \tag{5.19}$$

with Δm given by Eq. (5.17).

We have all the tools to compute the average $\Gamma_{\text{qu}} = \langle \gamma_{\text{qu}} \rangle$. It is given by

$$\begin{aligned}
\Gamma_{\text{qu}} &= \sum_{n,m} \gamma_{\text{qu}}[n, m] \, p[n, m] \\
&= \sum_{n,m} \left[\log p_n^i / p_m^i - \tau^2 \frac{\Delta m}{p_m^i} \right] \left[\delta_{mn} \, p_n^i + \tau^2 \, p_n^i \big(|\langle m|H|n \rangle|^2 - \delta_{mn} \langle n|H^2|n \rangle \big) \right] \\
&\approx \sum_{n,m} \left[\delta_{mn} \, p_n^i \, \log p_n^i / p_m^i - \tau^2 \, \delta_{mn} \, p_n^i \frac{\Delta m}{p_m^i} + \tau^2 p_n^i \, \log p_n^i / p_m^i \, |\langle m|H|n \rangle|^2 \right. \\
&\quad \left. - \tau^2 \delta_{mn} p_n^i \, \log p_n^i / p_m^i \, \langle n|H^2|n \rangle + \mathcal{O}\big(\tau^4\big) \right]. \tag{5.20}
\end{aligned}$$

As $\log(p_n^i / p_n^i) = \log 1 = 0$, the first and last terms disappear. Also, we have that

$$\begin{aligned}
\sum_m \Delta m &= \sum_m \langle m|H\rho_i^{th}H|m \rangle - p_m^i \langle m|H^2|m \rangle \\
&= \text{tr}\big\{ H\rho_i^{th}H \big\} - \text{tr}\big\{ \Delta[\rho_i^{th}]H^2 \big\} \\
&= \text{tr}\big\{ H^2(\rho_i^{th} - \Delta[\rho_i^{th}]) \big\} = 0, \tag{5.21}
\end{aligned}$$

because the initial state is already diagonal in the basis $\{|n\rangle\}$ ($\rho_i^{th} = \sum_n p_n^i |n\rangle\langle n|$). Hence, the final expression for Γ_{qu} is

$$\Gamma_{\text{qu}} = \tau^2 \sum_{n,m} p_n^i \, \log p_n^i / p_m^i |\langle m|H|n \rangle|^2. \tag{5.22}$$

If we now replace the populations by their expressions $p_n^i = \exp(-\beta\epsilon_m)/Z_i$, we get

$$\Gamma_{\text{qu}} = \beta\tau^2 \sum_{n,m} p_n^i (\epsilon_m - \epsilon_n) |\langle m|H|n \rangle|^2, \tag{5.23}$$

which is the exact same expression we obtained for the total entropy production (Eq. (3.35)).

This happens because the expression for γ_{qu} in Eq. (5.19) is exactly

$$\gamma_{\mathrm{qu}}[n, m] = \sigma[n, m] - \tau^2 \frac{\Delta m}{p_m^i}, \tag{5.24}$$

and the average of the second term, which we find corresponds to γ_{cl} (as $\sigma = \gamma_{\mathrm{qu}} + \gamma_{\mathrm{cl}}$), is identically zero. Therefore, in this particular case where the protocol is cyclic and the drive is applied for a short time τ, on average, the contribution from changes in populations of the system is null. Using the same argument, we will notice that all the cumulants of γ_{qu} will be equal to those of σ, for which we have already obtained a general expression for in Section 3.2.4. This indicates that, up to order $\mathcal{O}(\tau^2)$, all entropy production comes from γ_{qu}.

5.2.2 $H_f = H_i + \delta H$ and $\tau \to 0, U = 1$

In this case, we recall that $\rho_\tau = \rho_i^{th} = \sum_n p_n^i |n\rangle\langle n|$, and the final Hamiltonian is a perturbed version of the initial one, with basis $|n'\rangle$, where the eigenvector $|m'\rangle$ is given in Eq. (3.41). The populations of the final state $p_{m'}^\tau$ are given by

$$
\begin{aligned}
p_{m'}^\tau &= \langle m'|\rho_\tau|m'\rangle = \langle m'|U\rho_i^{th}U^\dagger|m'\rangle \approx \langle m'|\rho_i^{th}|m'\rangle \\[6pt]
&\approx \langle m'^{(0)}|\rho_i^{th}|m'^{(0)}\rangle + \langle m'^{(0)}|\rho_i^{th}|m'^{(1)}\rangle + \langle m'^{(1)}|\rho_i^{th}|m'^{(0)}\rangle + \langle m'^{(1)}|\rho_i^{th}|m'^{(1)}\rangle \\[6pt]
&\quad + \langle m'^{(0)}|\rho_i^{th}|m'^{(2)}\rangle + \langle m'^{(2)}|\rho_i^{th}|m'^{(0)}\rangle + \mathcal{O}(\delta H^3) \\[6pt]
&= p_m^i + \sum_{k\neq m} \frac{\langle k|\delta H|m\rangle}{\epsilon_m - \epsilon_k} \langle m|\rho_i^{th}|k\rangle + \sum_{k\neq m} \frac{\langle m|\delta H|k\rangle}{\epsilon_m - \epsilon_k} \langle k|\rho_i^{th}|m\rangle \\[6pt]
&\quad + \sum_{k\neq m}\sum_{\ell\neq m} \frac{\langle k|\delta H|m\rangle\langle m|\delta H|\ell\rangle}{(\epsilon_m - \epsilon_k)(\epsilon_m - \epsilon_\ell)} \langle k|\rho_i^{th}|\ell\rangle + \sum_{k\neq m}\sum_{\ell\neq m} \frac{\langle \ell|\delta H|k\rangle\langle m|\delta H|\ell\rangle}{(\epsilon_m - \epsilon_k)(\epsilon_m - \epsilon_\ell)} \langle m|\rho_i^{th}|k\rangle \\[6pt]
&\quad + \sum_{k\neq m} \frac{\langle m|\delta H|n\rangle\langle m|\delta H|k\rangle}{(\epsilon_m - \epsilon_k)^2} \langle m|\rho_i^{th}|k\rangle - \frac{1}{2}\sum_{k\neq m} \frac{|\langle m|\delta H|k\rangle|^2}{(\epsilon_m - \epsilon_k)^2} p_m^i \\[6pt]
&\quad + \sum_{k\neq m}\sum_{\ell\neq m} \frac{\langle k|\delta H|\ell\rangle\langle \ell|\delta H|m\rangle}{(\epsilon_m - \epsilon_k)(\epsilon_m - \epsilon_\ell)} \langle k|\rho_i^{th}|m\rangle + \sum_{k\neq m} \frac{\langle m|\delta H|m\rangle\langle k|\delta H|m\rangle}{(\epsilon_m - \epsilon_k)^2} \langle k|\rho_i^{th}|m\rangle \\[6pt]
&\quad - \frac{1}{2}\sum_{k\neq m} \frac{|\langle m|\delta H|k\rangle|^2}{(\epsilon_m - \epsilon_k)^2} p_m^i \\[6pt]
&= p_m^i + \sum_{k\neq m}\sum_{\ell\neq m} \frac{\langle k|\delta H|m\rangle\langle m|\delta H|\ell\rangle}{(\epsilon_m - \epsilon_k)(\epsilon_m - \epsilon_\ell)} \langle k|\rho_i^{th}|\ell\rangle - \sum_{k\neq m} \frac{|\langle m|\delta H|k\rangle|^2}{(\epsilon_m - \epsilon_k)^2} p_m^i. \tag{5.25}
\end{aligned}
$$

In this last step, we have considered the fact that ρ_i^{th} is diagonal in the $\{|m\rangle\}$ basis, and so every term that depends on $\langle k|\rho_i^{th}|m\rangle$, for $k \neq m$, is zero. For this same reason, the first term that depends on δH^2 has to be considered only for $k = \ell$. So, the final result is

$$p_{m'}^{\tau} = p_m^i + \sum_{k \neq m} |h_{mk}|^2 (p_k^i - p_m^i),\tag{5.26}$$

with $|h_{mk}|^2$ given by Eq. (3.49). Now, we can write $\gamma_{\text{qu}}[n, m'] = \log p_n^i - \log p_{m'}^{\tau}$ as

$$\gamma_{\text{qu}}[n, m'] = \log p_n^i - \log \left\{ p_m^i + \sum_{k \neq m} |h_{mk}|^2 (p_k^i - p_m^i) \right\}$$

$$= \log p_n^i - \log \left\{ p_m^i \left[1 + \sum_{k \neq m} |h_{mk}|^2 (p_k^i / p_m^i - 1) \right] \right\}.\tag{5.27}$$

Again, using the approximation $\log(1 + x) \approx x$, for $x \ll 1$, we have

$$\gamma_{\text{qu}}[n, m'] = \log p_n^i / p_m^i - \sum_{k \neq m} |h_{mk}|^2 (p_k^i / p_m^i - 1).\tag{5.28}$$

In posession of this last result, together with Eq. (3.48), we compute the average value Γ_{qu}.

$$\Gamma_{\text{qu}} = \sum_{n,m'} \gamma_{\text{qu}}[n, m'] \ P[n, m']$$

$$= \sum_{n} \left(\gamma_{\text{qu}}[n, n'] \ p_{n'|n} \ p_n^i + \sum_{m \neq n} \gamma_{\text{qu}}[n, m'] \ p_{m'|n} \ p_n^i \right)$$

$$= \sum_{n} \left\{ -\sum_{k \neq n} |h_{nk}|^2 (p_k^i / p_n^i - 1) \left[p_n^i - p_n^i \sum_{k \neq n} |h_{nk}|^2 \right] \right.$$

$$\left. + \sum_{m \neq n} |h_{mn}|^2 \ p_n^i \left[\log p_n^i / p_m^i - \sum_{k \neq m} |h_{mk}|^2 (p_k^i / p_m^i - 1) \right] \right\}.\tag{5.29}$$

Approximating up to order $\mathcal{O}(\delta H^2)$, as we have done all the way up to this point, we have

$$\Gamma_{\text{qu}} = \sum_{n} \left[\sum_{m \neq n} |h_{mn}|^2 \ p_n^i \ \log p_n^i / p_m^i - \sum_{k \neq n} |h_{nk}|^2 (p_k^i - p_n^i) \right].\tag{5.30}$$

As the matrix h is hermitian and $p_k^i - p_n^i$ is odd when exchanging n and k, the second term on

Eq. (5.30) vanishes. The final result is

$$\Gamma_{\text{qu}} = \sum_n \sum_{m \neq n} |h_{mn}|^2 \, p_n^i \log p_n^i / p_m^i. \tag{5.31}$$

If we substitute the expressions for the initial populations inside the logarithm, we obtain

$$\Gamma_{\text{qu}} = \beta \sum_n \sum_{m \neq n} |h_{mn}|^2 \, p_n^i (\epsilon_m - \epsilon_n). \tag{5.32}$$

Looking at the final expressions for Γ_{qu} of the two cases studied above (Eqs (5.23) and (5.32)), we can't help but notice they are very similar. In the first case, we take the initial state, apply a unitary during a short period of time, that rotates the eigenbasis of the state of the system. In the end, we measure it in the original energy basis. In the second case, we take the same initial state and simply measure it in a different basis, the detuned basis.

Figure 5.1: Comparison between the two limiting cases: in the first case, the system's state is rotated and the basis is fixed; in the second, the basis is rotated in the other direction, and the state remains fixed. The projection of the state into the basis ends up being the same in both cases.

We can think of this problem as if, in the first case, we rotate the state to one side, then measure it in a fixed basis, and in the second case we rotate the basis to the other side and keep a fixed state (see Figure 5.1). The "angle" between the state and the basis is the same, so the "projection" gives the same value. But the process is different. The same does not happen for the total entropy production, however. In Appendix D we develop the analytical expression for the case of a single qubit using the macrospin model.

5.3 Numerical applications

5.3.1 Macrospin model

We proceed to analyse some numerical results of the probability distribution of γ_{qu}. First, we will consider the macrospin model proposed in Sec. 4.1. Similarly to Sec. 4.1.2, we set

$h_z = 1$. The results are shown in Fig. 5.2 for different values of d.
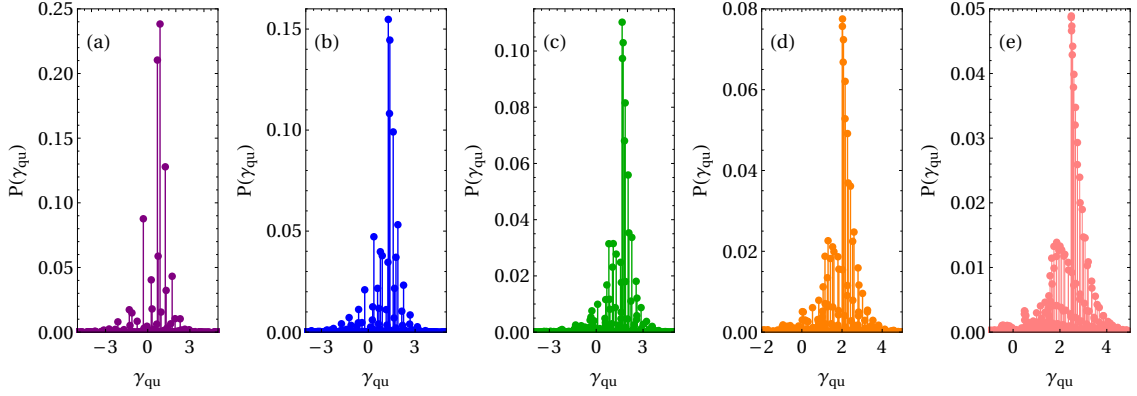
Figure 5.2: Probability distributions of γ_{qu} for different values of d for the macrospin model. Other parameters are fixed: $\beta = 1$, $\tau = 1$ and $h_x = 0.5$. Images (a) through (e) have $d = 20, 50, 100, 200$ and 500, respectively.
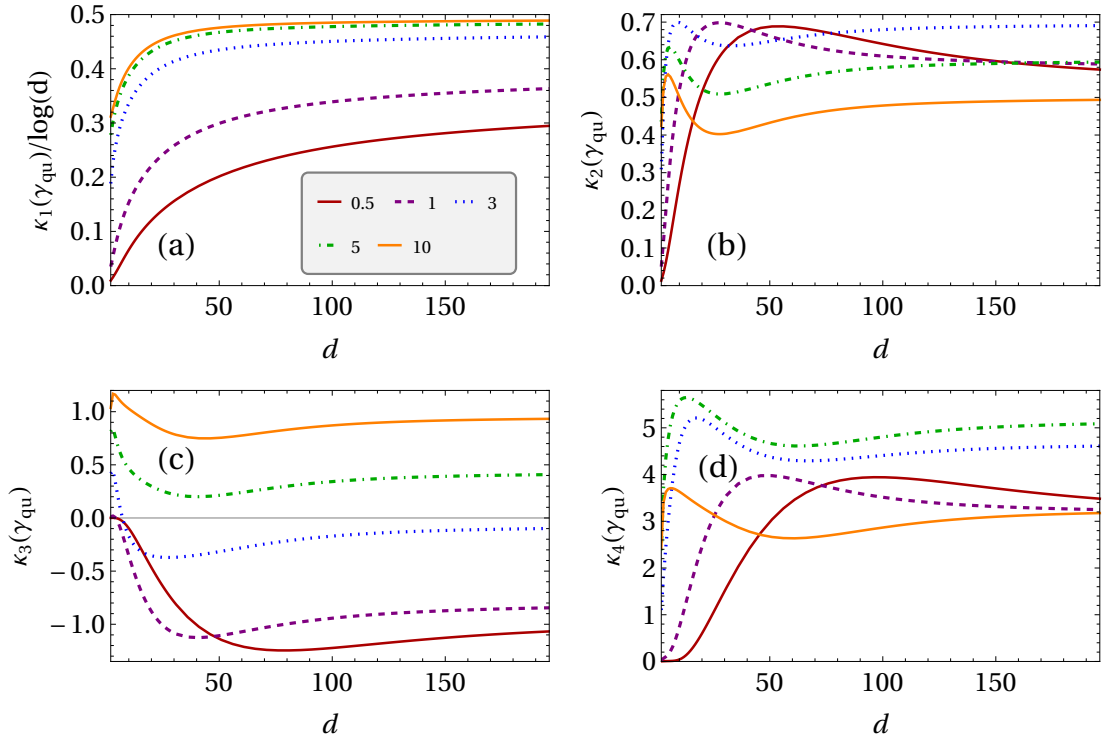
Figure 5.3: Cumulants of γ_{qu} as a function of the dimension d for different values of β (macrospin model). Image (a) is scaled by $\log(d)$. Other parameters are fixed: $\tau = 1$ and $h_x = 0.5$.

First, from Figure 5.2, we notice that, differently from the total entropy production (Fig. 4.2), it does not seem that the probability distribution tends to a Gaussian even for dimensions as high as 500. This could be due to the fact that the cumulants are not extensive (they do not depend linearly on the dimension); instead, they seem to saturate for finite dimension, except for the mean, which grows with $\log(d)$ (Fig. 5.3). Because of that, extremely large dimensions may be necessary to observe a Gaussian behavior [5].

It would also be expected that, for $d \rightarrow \infty$, the system would behave as a classical macrospin [60], and that therefore the quantum contribution to the entropy production should, at least on average, tend to zero. However, from Fig 5.3 (a), it is evident that the average increases as d grows larger. This is due to the fact that, even though d is large, we still assume we have full resolution to access all of the system's eigenstates [5]. This would probably be different if some sort of coarse graining of the energy levels was used.

Figure 5.4: Probability distributions of γ_{qu} for different values of β for the macrospin model. Plots (a) through (c) have $\beta = 0.1, 0.5, 1, 5$ and 50, respectively. Other parameters are fixed: $d = 100$, $\tau = 1$ and $h_x = 0.5$.
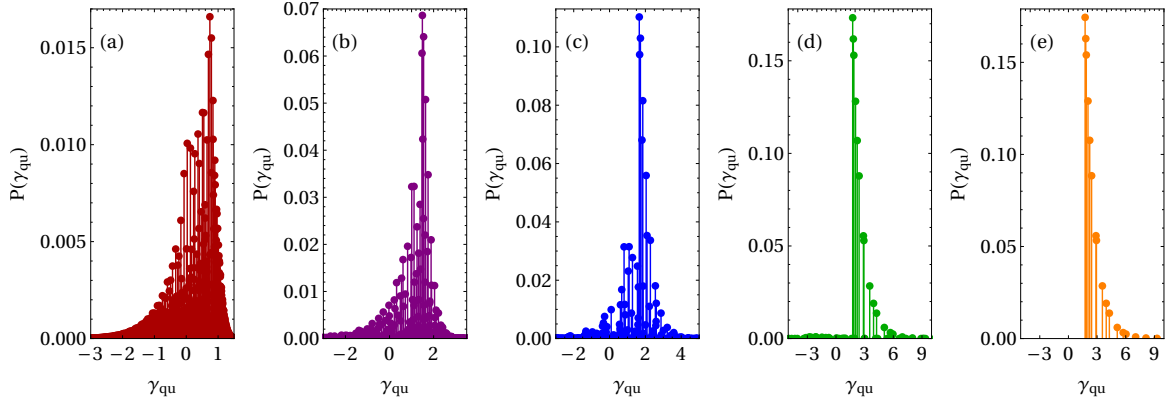

Figure 5.5: Cumulants of γ_{qu} as a function of β for different values of d (macrospin model). Other parameters are fixed: $\tau = 1$ and $h_x = 0.5$.

Figures 5.4 and 5.5 depict the probability distributions and corresponding cumulants for different values of β. Differently than the total entropy production (Fig 4.7), we notice from Fig. 5.5 that, for large β (small temperature), the cumulants already approach a constant, i.e., they do not depend on β.

As for the total entropy production, the dependence on τ and h_x is not simple (results not shown).

5.3.2 LMG model

Now we turn to the analysis of the distribution of γ_{qu} in the LMG model. Figures 5.6 and 5.7 present the first four cumulants as a function of g, from which the emergence of the phase transition is clearly observed. In this case, differently than for the total entropy production (Figs. 4.12 and 4.13), the dependence with d and β does not follow a simple scaling law, and therefore we include this analysis in Figures 5.8 and 5.9.
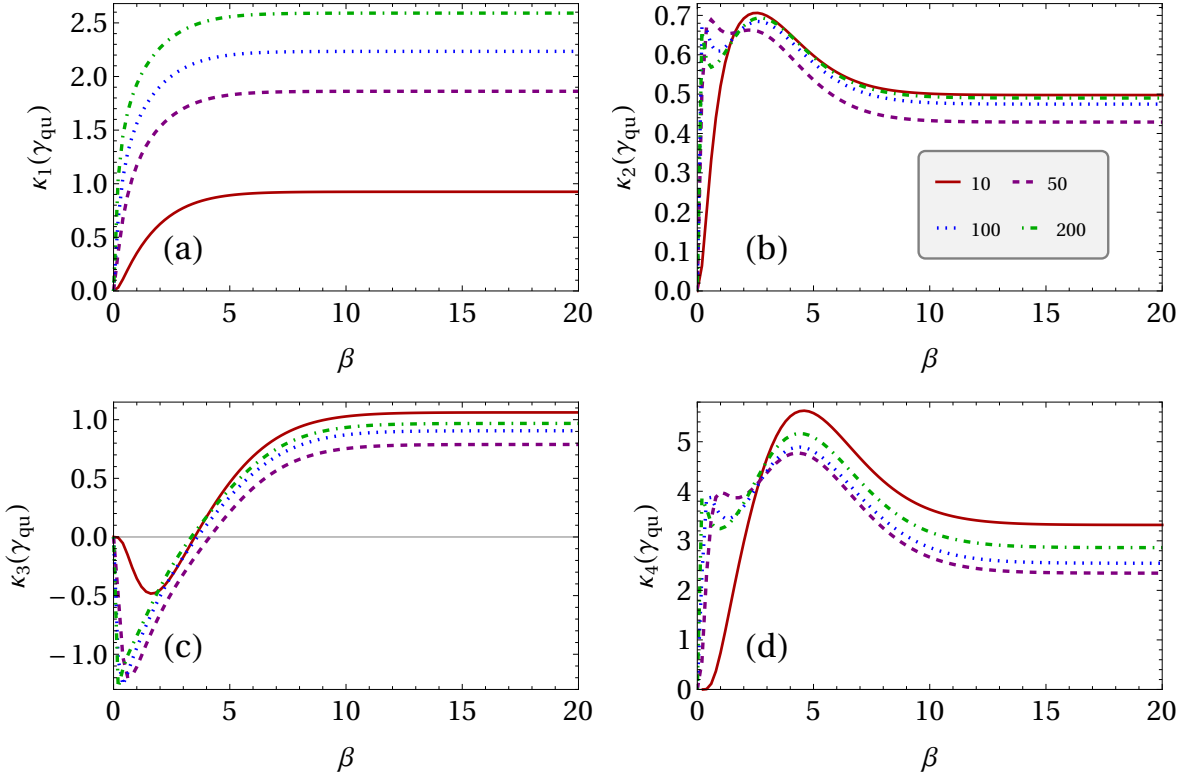

Figure 5.6: Cumulants of γ_{qu} as a function of g for different values of d (LMG model). Other parameters are fixed: $\beta = 10$ and $\delta g = 0.01$.

From Figure 5.8, it seems that the first two cumulants (images (a) and (b)) depend in a logarithmic scale with the dimension. For the third and fourth cumulants ((c) and (d)), they

Figure 5.7: Cumulants of γ_{qu} as a function of g for different values of β (LMG model). Other parameters are fixed: $d = 500$ and $\delta g = 0.01$.

appear to saturate with the dimension. It is possible that the two first cumulants do saturate, but that happens at extremely high dimension. In this manner, it differs from the macrospin model, that, for all cumulants except for the first, does not depend on d for higher dimensions.

Again, as in the macrospin model, we note that the average $\kappa_1(\gamma_{qu}) = \Gamma_{qu}$ does not vanish for large dimensions, as would be expected if it reached a classical limit. The explanation in the same given in Sec. 5.3.1.

Turning our attention to Figure 5.7, it seems that, for higher β, the cumulants do not depend on the temperature anymore, similarly to the macrospin model. Indeed, looking at Fig. 5.9, this seems to be the case, except that, for larger dimensions, it looks that a much larger β is needed in order for the cumulant to saturate.

Figure 5.8: Cumulants of γ_{qu} as a function of d for different values of β (LMG model). Other parameters are fixed: $g = 0.9$ and $\delta g = 0.01$.
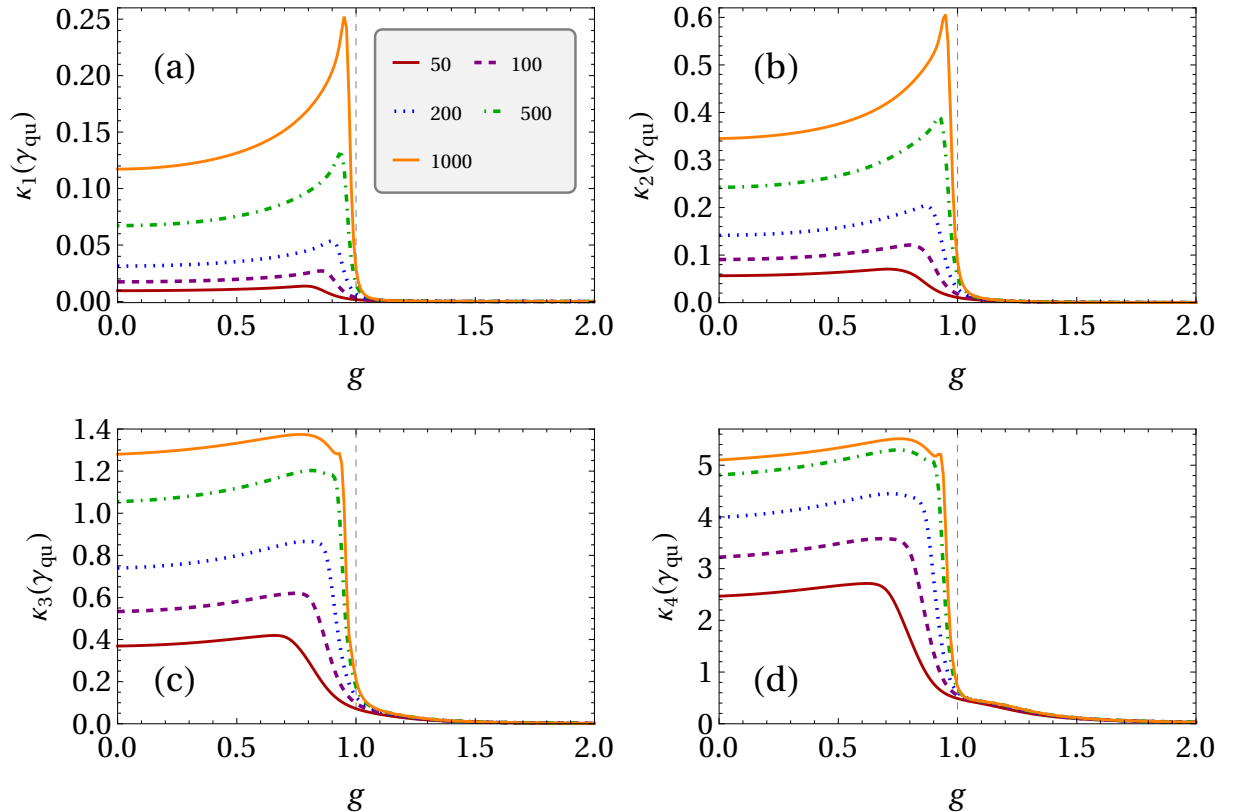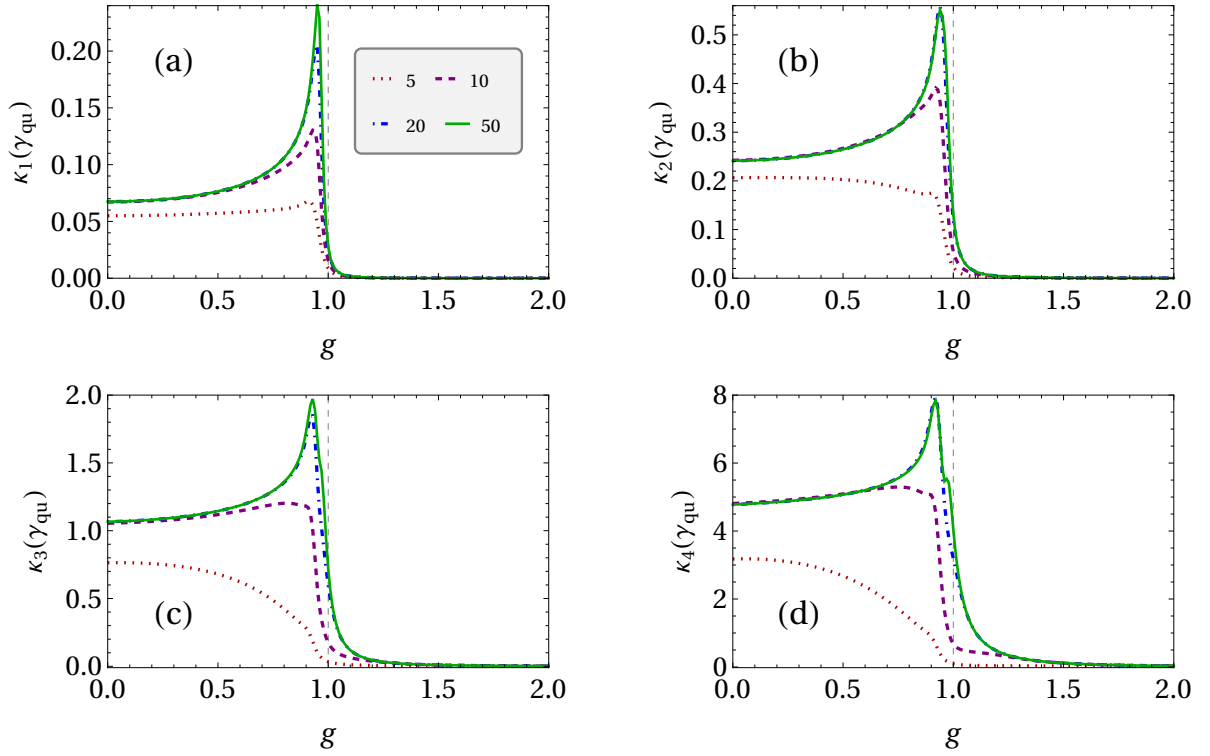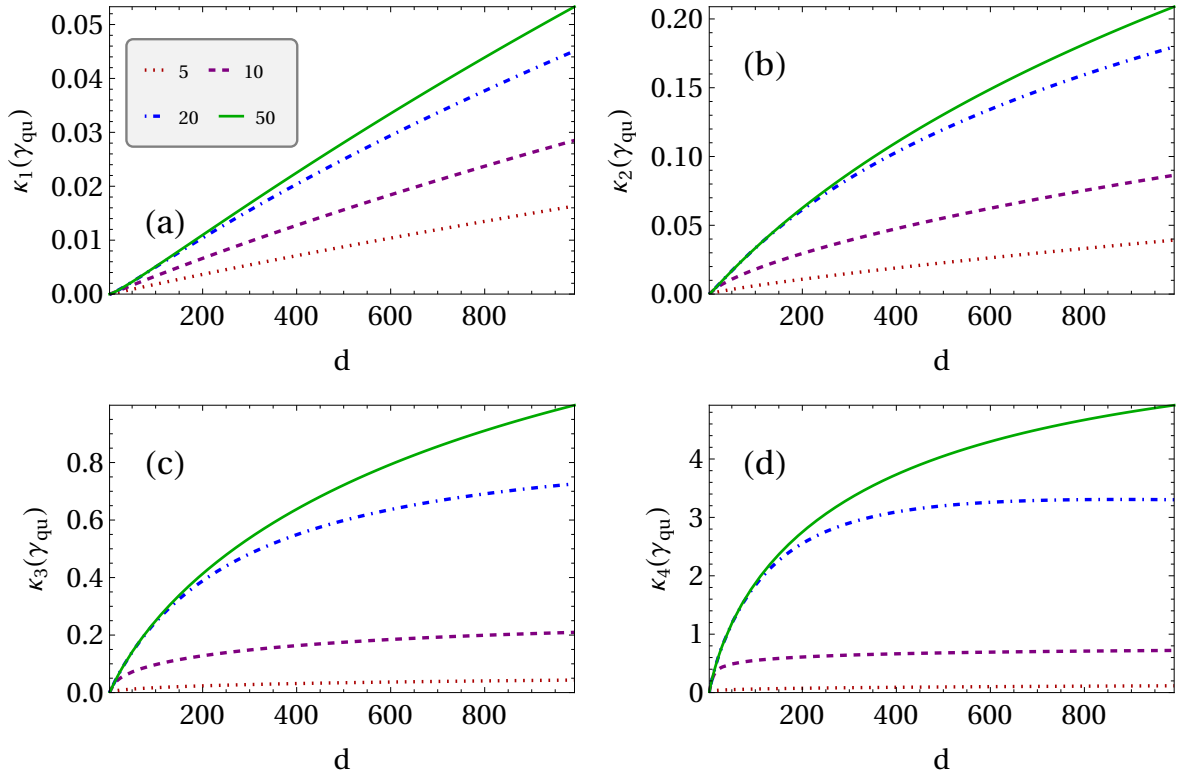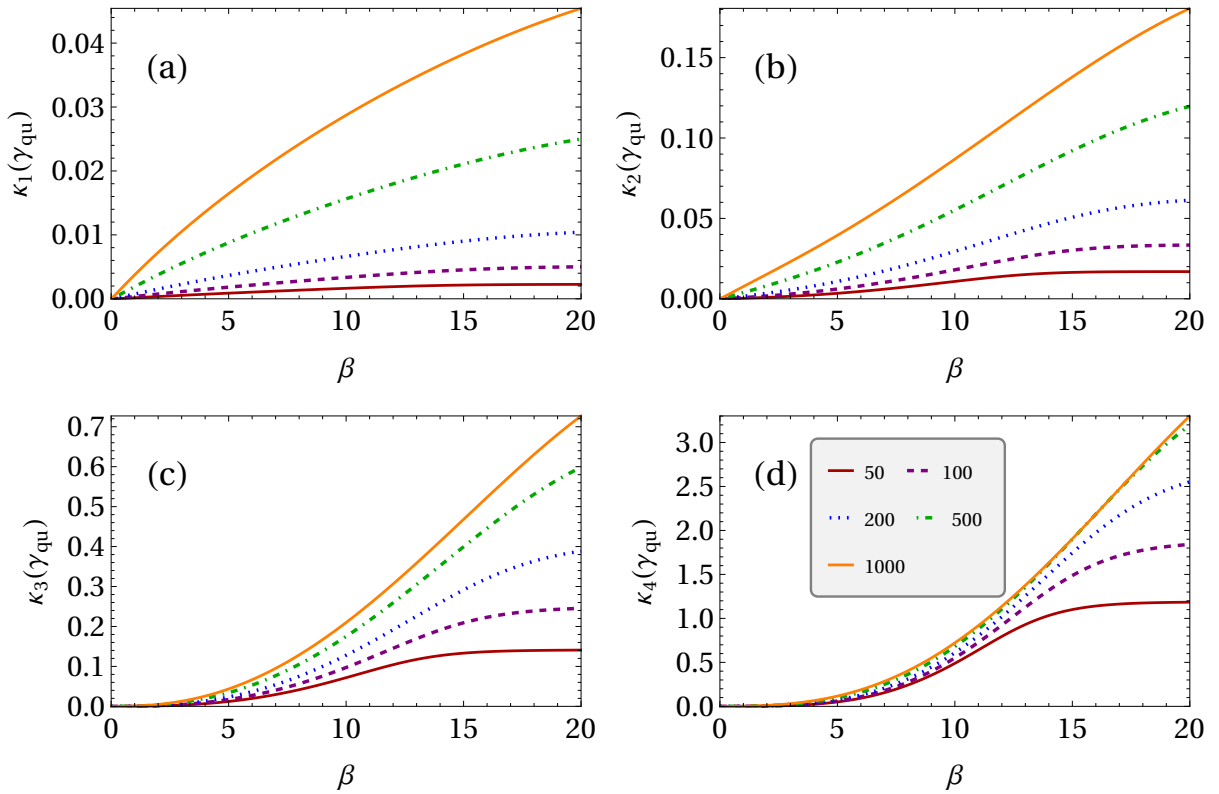

Figure 5.9: Cumulants of γ_{qu} as a function of β for different values of d (LMG model). Other parameters are fixed: $g = 0.9$ and $\delta g = 0.01$.

Chapter 6

Coherent contribution to entropy production: Λ splitting

The overarching goal of this dissertation is to understand how coherences and populations contribute to the entropy, specially at the stochastic level. However, the splitting presented in the previous chapter is not unique.

In this chapter, we will present an alternative splitting, which allows for a different interpretation of the roles of quantum and classical effects. The splitting was introduced in Ref. [5], and was motivated by results from [4]. In Ref. [4], the authors studied the statistics of the dissipated work w_{diss} (which is directly related to the entropy production by $\Sigma = \beta w_{\text{diss}}$) in infinitesimal quench protocols. They concluded that it is possible to derive a fluctuation-dissipation relation for it, that is valid if the Hamiltonian commutes with itself at all times, but that a quantum correction arises if this is not the case. That is, the authors state that the quantum contribution to the statistics comes from coherent part of the final Hamiltonian. In Reference [5], the proposed splitting generalized to non-infinitesimal quenches, and both splittings were compared in detail. This chapter will focus on this new splitting, both in the average level as well as in the stochastic level, and analyse some numerical results.

The work protocol will again be the same as in Sec. 3.2.2. This time, instead of splitting the protocol by considering the intermediate state $\Delta_f[\rho_\tau]$, we will consider that the final Hamiltonian is dephased in the basis of ρ_τ. That is, considering $\rho_\tau = U \rho_i^{th} U^\dagger = \sum_n p_n^i |\tilde{n}\rangle\langle\tilde{n}|$, where $|\tilde{n}\rangle = U |n\rangle$, the dephased Hamiltonian is defined as

$$\Delta_\tau[H_f] := \sum_{\tilde{n}} |\tilde{n}\rangle\langle\tilde{n}| H_f |\tilde{n}\rangle\langle\tilde{n}|, \tag{6.1}$$

and the intermediate state $\tilde{\rho}_f^{th}$ is defined as [5]

$$\tilde{\rho}_f^{th} = \frac{e^{-\beta \Delta_\tau [H_f]}}{\text{tr}\big(e^{-\beta \Delta_\tau [H_f]}\big)} = \sum_{\tilde{n}} \tilde{p}_n^f \, |\tilde{n}\rangle\langle\tilde{n}| \, , \tag{6.2}$$

where $\tilde{p}_n^f = \exp(-\beta \langle\tilde{n}|H_f|\tilde{n}\rangle)/Z_{\Delta_\tau [H_f]}$, with $Z_{\Delta_\tau [H_f]} = \text{tr}\{\exp(-\beta \Delta_\tau [H_f])\}$. This intermediate state can be intuitively explained when considering an infinitesimal quench from H_i to $H_f = H_i + \delta H$, with $U \to 1$ [4]. In this particular case, $\rho_\tau = \rho_i^{th}$ and their eigenbasis is the same as that of H_i, so the dephased final Hamiltonian $\Delta_\tau [H_f]$ is actually dephased with respect to the basis of H_i. In this case, the protocol can be divided into two quenches: the first, $H_i \to \Delta_\tau [H_f]$, and the second, $\Delta_\tau [H_f] \to H_f$. The first quench only changes the populations of the system, as the basis of both Hamiltonians are the same. The second produces coherences in the state, because the basis is rotated [4, 5]. Here, we will consider the general case where the unitary is not the identity, but we will keep this concept in mind when separating the contributions from populations and coherences.

Finally, the total entropy production $\Sigma = S(\rho_\tau || \rho_f^{th})$ is divided into two contributions,

$$\Sigma = \Lambda_{\text{qu}} + \Lambda_{\text{cl}}, \tag{6.3}$$

given by [5]

$$\Lambda_{\text{qu}} := \text{tr}\big[\rho_\tau (\log \tilde{\rho}_f^{th} - \log \rho_f^{th})\big], \tag{6.4}$$

$$\Lambda_{\text{cl}} := S(\rho_\tau || \tilde{\rho}_f^{th}). \tag{6.5}$$

The classical term, Λ_{cl}, compares states ρ_τ and $\tilde{\rho}_f^{th}$, which have the same eigenbasis and therefore differ only in terms of populations, as desired. On the other hand, Λ_{qu} compares $\tilde{\rho}_f^{th}$, that is diagonal in the basis of the dephased Hamiltonian, and ρ_f^{th}, that has the basis of H_f as its eigenbasis, and therefore it accounts for changes in the system due to basis rotation. In this case, the classical term can also be written as a relative entropy, as the terms of the $\Gamma-$splitting (Eqs. (5.3) and (5.4)); because of that, it is clear that $\Lambda_{\text{cl}} \geq 0$. As for Λ_{qu}, first let us rewrite it

in terms of free-energies. We have that

$$\Lambda_{\mathrm{qu}} = \mathrm{tr}\big[\rho_\tau(\log \tilde{\rho}_f^{th} - \log \rho_f^{th})\big]$$

$$= \mathrm{tr}\big[\rho_\tau(-\beta\Delta_\tau[H_f] - \log Z_{\Delta_\tau[H_f]} + \beta H_\tau + \log Z_f)\big]$$

$$= \mathrm{tr}[\beta\rho_\tau(H_f - \Delta_\tau[H_f])] + \mathrm{tr}\{\beta[F(\tilde{\rho}_f^{th}) - F(\rho_f^{th})]\}, \tag{6.6}$$

where $F(\tilde{\rho}_f^{th}) = -T\log Z_{\Delta_\tau[H_f]}$ and $F(\rho_f^{th}) = -T\log Z_f$. Now, we notice that the subtraction of Hamiltonians in the first term results in the coherent part of H_f, that is, it has no diagonal elements, and therefore the first trace is zero. The final result is thus

$$\Lambda_{\mathrm{qu}} = \mathrm{tr}\{\beta[F(\tilde{\rho}_f^{th}) - F(\rho_f^{th})]\}. \tag{6.7}$$

Even in this form it is not obvious that $\Lambda_{\mathrm{qu}} \geq 0$, but in Ref. [5] we have shown that this is in fact the case. The proof is based on the Bogoliubov variational theorem [11], which in this case states that

$$F(\rho_f^{th}) \leq F(\tilde{\rho}_f^{th}) + \mathrm{tr}\big(\tilde{\rho}_f^{th} H_f^c\big), \tag{6.8}$$

where $H_f^c = H_f - \Delta_\tau[H_f]$ is the coherent part of the final Hamiltonian. But, as we have already argued, the trace of the second term will be null, and therefore $F(\tilde{\rho}_f^{th}) - F(\rho_f^{th}) \geq 0$, which confirms that $\Lambda_{\mathrm{qu}} \geq 0$.

6.1 Stochastic trajectories

As in the case of the Γ-splitting, we may formulate the theory for the Λ-splitting at the stochastic level. The only difference is that, instead of comparing the populations of initial and final thermal states with that of the final state ρ_τ dephased in the basis of H_f, we consider the populations $\tilde{p}_n^f = \exp(-\beta\langle\tilde{n}|H_f|\tilde{n}\rangle)/Z_{\Delta_\tau[H_f]}$ of the state $\tilde{\rho}_f^{th}$ presented in Eq. (6.2), that is the thermal state of the final Hamiltonian dephased in the basis of ρ_τ. The stochastic quantum and classical contributions are given by [5]

$$\lambda_{\mathrm{qu}}[n, m'] := \log \tilde{p}_n^f - \log p_{m'}^f, \tag{6.9}$$

$$\lambda_{\mathrm{cl}}[n, m'] := \log p_n^i - \log \tilde{p}_n^f. \tag{6.10}$$

These quantities sum up to $\sigma[n, m'] = \log p_n^i - \log p_{m'}^f$, as expected. Also, we can show that their averages correspond to Λ_{qu} and Λ_{cl}. Again, with $P[n, m'] = |\langle m'|U|n\rangle|^2 \, p_n^i$, the average of $\lambda_{\mathrm{qu}}[n, m']$ is given by

$$
\begin{aligned}
\langle \lambda_{\mathrm{qu}}[n, m'] \rangle &= \sum_{n, m'} \lambda_{\mathrm{qu}}[n, m'] P[n, m'] \\
&= \sum_{n, m'} |\langle m'|U|n\rangle|^2 \, p_n^i [\log \tilde{p}_n^f - \log p_{m'}^f] \\
&= \sum_n p_n^i \log \tilde{p}_n^f - \sum_{m'} p_{m'}^\tau \log p_{m'}^f.
\end{aligned}
\tag{6.11}
$$

In the second term, both populations are given in the basis $\{|m'\rangle\}$, so we can simply rewrite it as $\sum_{m'} p_{m'}^\tau \log p_{m'}^f = \mathrm{tr}(\rho_\tau \log \rho_f^{th})$. As for the first term, we can rewrite the populations of the initial state as $p_n^i = \langle n|\rho_i^{th}|n\rangle = \langle \tilde{n}|U\rho_i^{th}U^\dagger|\tilde{n}\rangle = \langle \tilde{n}|\rho_\tau|\tilde{n}\rangle$, which leads to $\sum_n p_n^i \log \tilde{p}_n^f = \mathrm{tr}(\rho_\tau \log \tilde{\rho}_f^{th})$. Therefore, $\langle \lambda_{\mathrm{qu}}[n, m'] \rangle = \Lambda_{\mathrm{qu}}$, as expected.

In the case of $\lambda_{\mathrm{cl}}[n, m']$, we have that

$$
\begin{aligned}
\langle \lambda_{\mathrm{cl}}[n, m'] \rangle &= \sum_{n, m'} \lambda_{\mathrm{cl}}[n, m'] P[n, m'] \\
&= \sum_{n, m'} |\langle m'|U|n\rangle|^2 \, p_n^i [\log p_n^i - \log \tilde{p}_n^f] \\
&= \sum_n p_n^i [\log p_n^i - \log \tilde{p}_n^f] \\
&= \mathrm{tr}\big[\rho_i^{th}(\log \rho_i^{th} - \log \tilde{\rho}_f^{th})\big] \\
&= S(\rho_i^{th}||\tilde{\rho}_f^{th}) \\
&= \Lambda_{\mathrm{cl}}.
\end{aligned}
\tag{6.12}
$$

Just like γ_{qu} and γ_{cl} (Appendix B), λ_{cl} also satisfies a Jarzynski's equality [52]: $\langle e^{-\lambda_{\mathrm{cl}}} \rangle = 1$. However, the same is not true for λ_{qu}. Instead, as shown in Appendix E, one finds that $\langle e^{-\lambda_{\mathrm{qu}}} \rangle = \mathrm{tr}\{\rho_f^{th}(\tilde{\rho}_f^{th})^{-1}\rho_\tau\}$, which cannot be further simplified for a general unitary process. The quantum contribution only satisfies a fluctuation theorem in the case of a infinitesimal quench ($U \to 1$ and $H_f = H_i + \delta H$) [5].

6.2 Numerical applications

In this section we repeat the analysis of Sec. 5.3, but for the new splitting Λ.

6.2.1 Macrospin model
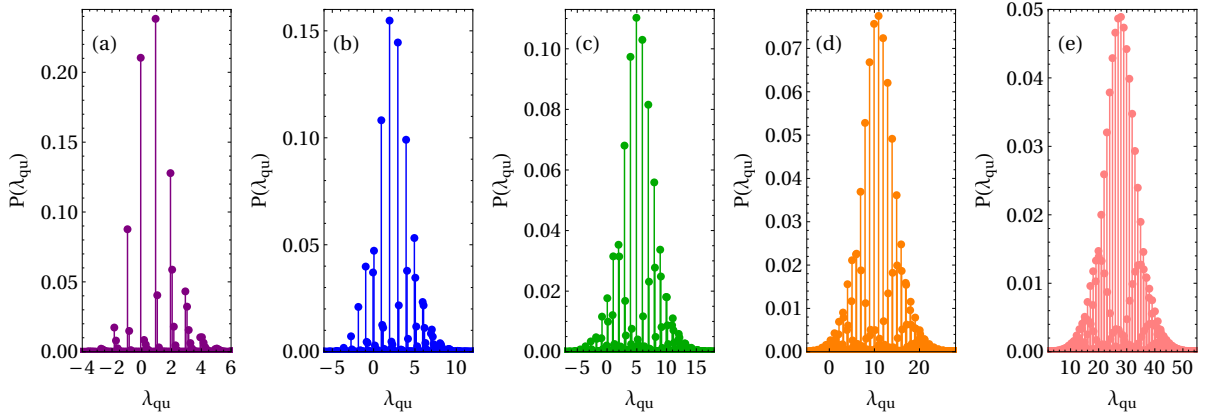
Figure 6.1: Probability distributions of λ_{qu} for different values of d. Other parameters are fixed: $\beta = 1$, $\tau = 1$ and $h_x = 0.5$. Images (a) through (e) have $d = 20, 50, 100, 200$ and 500, respectively.

In Figure 6.1 are shown the probability distributions of λ_{qu} for different values of dimension. Again, we set $h_z = 1$ for all the simulations. Just from that image, it seems that the distribution of λ_{qu} will not tend to a Gaussian, just like γ_{qu}. However, from Figure 6.2 we notice that for higher values of β it does behave like a Gaussian for sufficiently large d. For lower β, it may be necessary to go to even larger dimensions to reach a Gaussian probability distribution. But, in this manner, it seems that λ_{qu}'s behavior is more similar to that of the total entropy production (Fig. 4.2) than to γ_{qu} (Fig. 5.2).
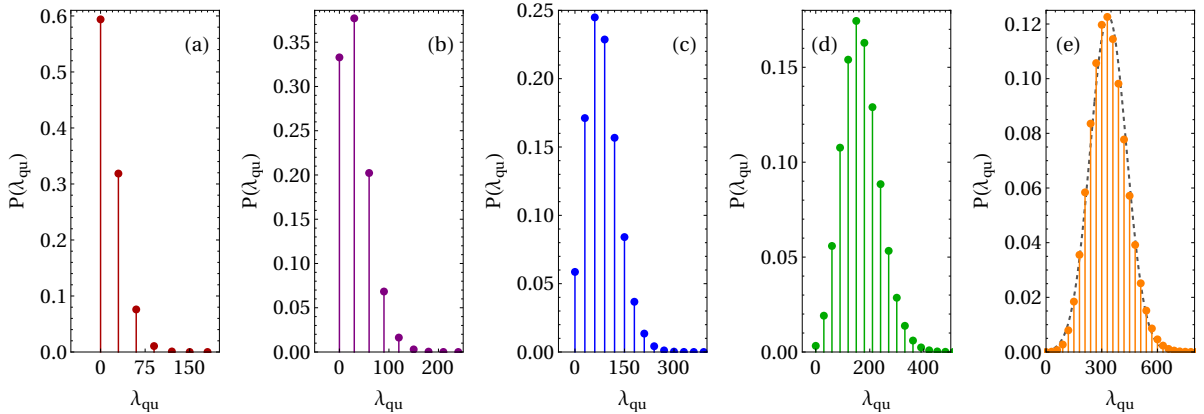

Figure 6.2: Probability distributions of λ_{qu} for different values of d for the macrospin model. Other parameters are fixed: $\beta = 30$, $\tau = 1$ and $h_x = 0.5$. Images (a) through (e) have $d = 10, 20, 50, 100$ and 200, respectively. In (e), the dashed gray curve represents a Gaussian with same average and standard deviation as the corresponding probability distribution.

Indeed, the behavior of the cumulants of λ_{qu} in Fig. 6.3 is very similar to that of the total entropy production depicted in Fig. 4.3. All the cumulants grow linearly with the dimension. Again, it is noticeable that the quantum contribution does not vanish for large dimensions, as happened with γ_{qu} (Sec. 5.3.1).
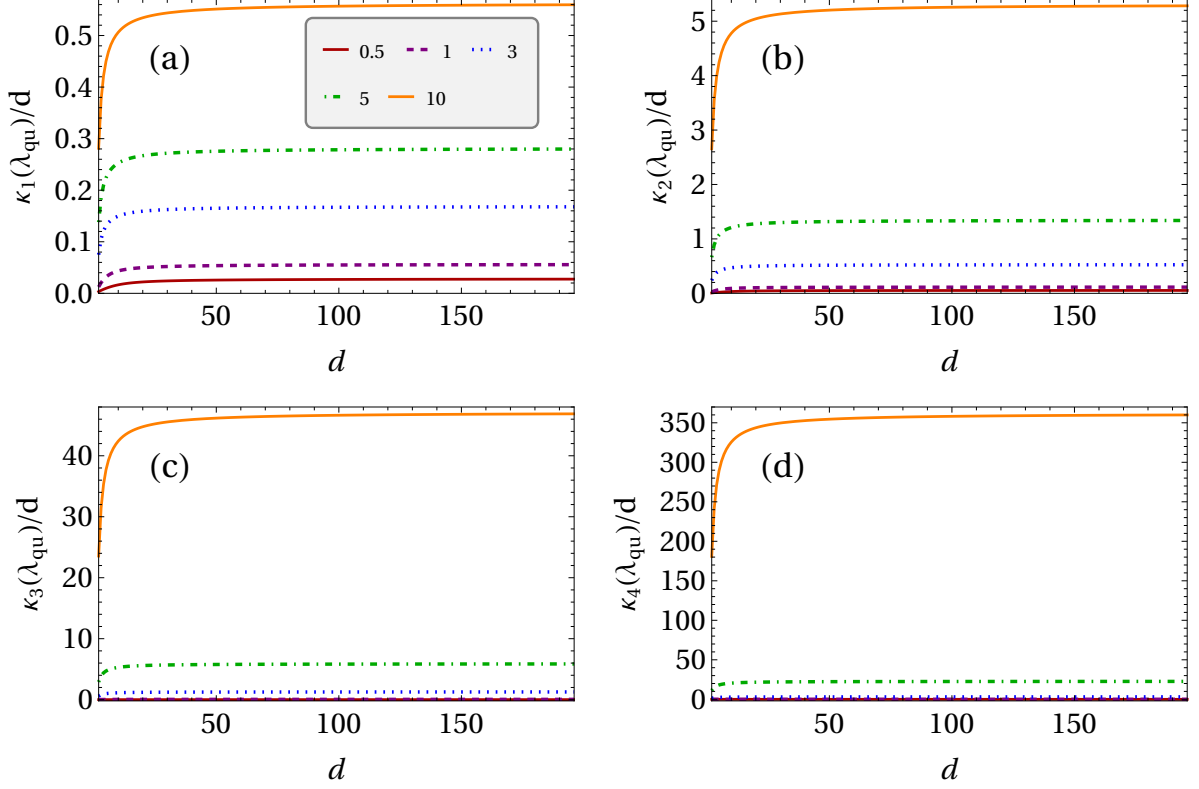
Figure 6.3: Cumulants of λ_{qu} as a function of the dimension d for different values of β (macrospin model). Image (a) is scaled by $\log(d)$. Other parameters are fixed: $\tau = 1$ and $h_x = 0.5$.

From the linear dependence on d, it becomes evident that the same argument of fine-graining used for γ_{qu} (Sec. 5.3.1) applies for λ_{qu}; even if we consider λ_{qu} to be the quantum contribution to the entropy production, it does not vanish for higher dimensions, because we still consider that we have access to all the degrees of freedom of the system.

Figure 6.4 shows probability distributions for different values of β. By looking at Fig. 6.5, we notice that, in a similar manner to what happens for the total entropy production, the dependence of λ_{qu} with β is proportional to β^n, for the cumulant of n-th order.

Finally, the dependence with τ and h_x is again oscillatory (results now shown).
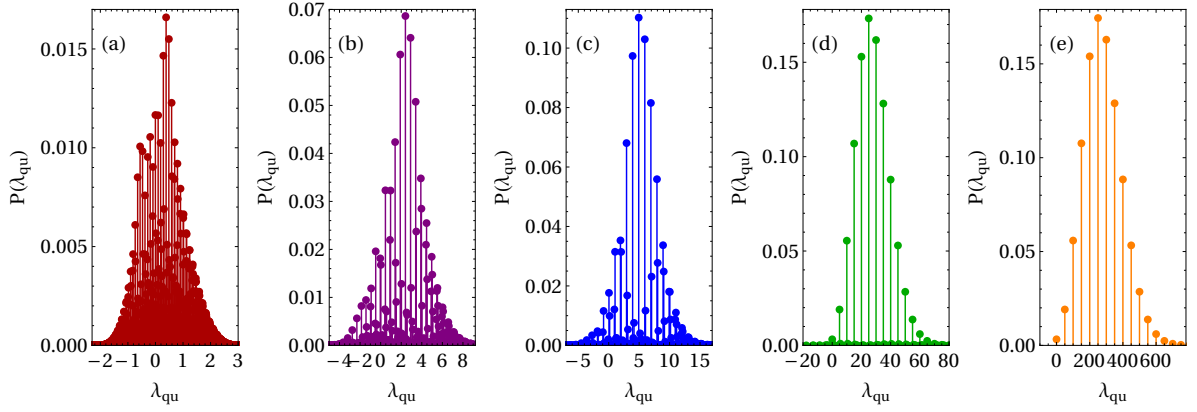
Figure 6.4: Probability distributions of λ_{qu} for different values of β for the macrospin model. Plots (a) through (c) have $\beta = 0.1, 0.5, 1, 5$ and 50, respectively. Other parameters are fixed: $d = 100$, $\tau = 1$ and $h_x = 0.5$.
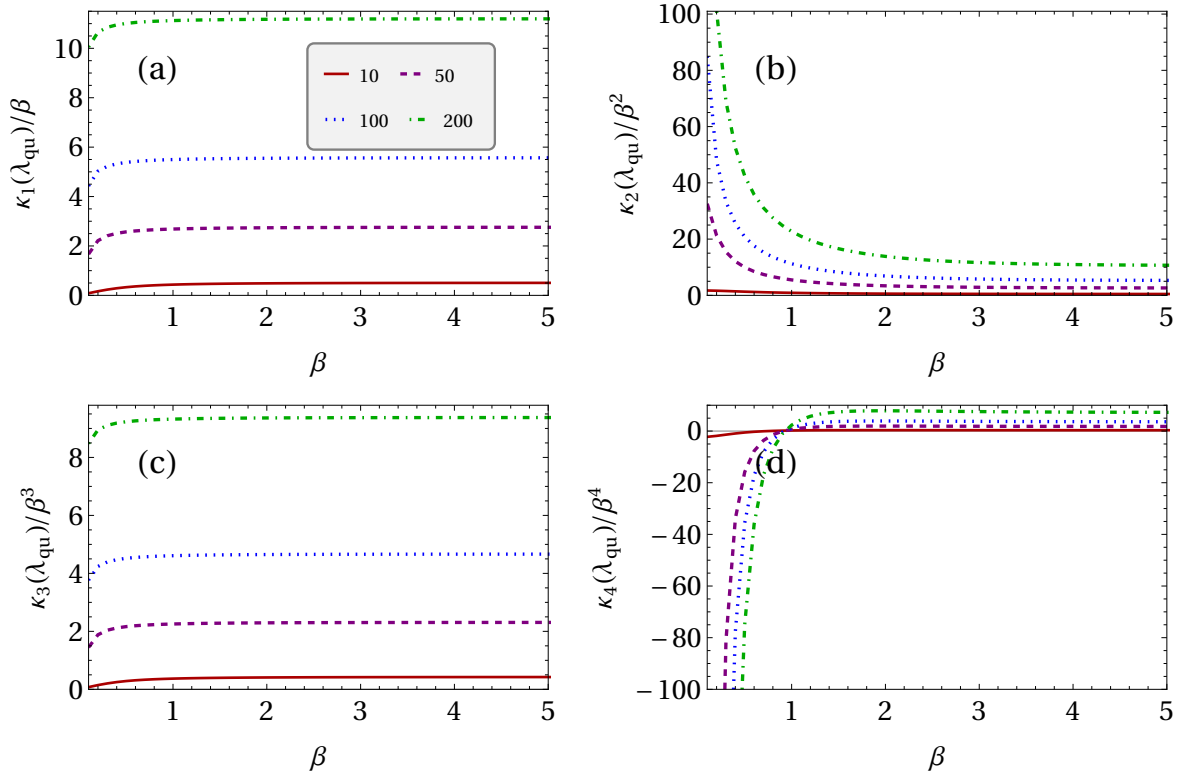
Figure 6.5: Cumulants of λ_{qu} as a function of β for different values of d (macrospin model). Other parameters are fixed: $\tau = 1$ and $h_x = 0.5$.

6.2.2 LMG model

At last, we turn ourselves to how λ_{qu} behaves on the LMG model. The plots of the first four cumulants against the parameter g are shown on Figure 6.6 for multiple values of dimension d and on Figure 6.7 for multiple values of the inverse temperature β. Both of the Figures are very similar to their versions for the total entropy production (Fig. 4.12 and 4.13).

We notice that the dependence with the d and β is again the same as for the macrospin model (Sec. 6.2.1): the cumulants depend linearly on d and with simple powers of β.
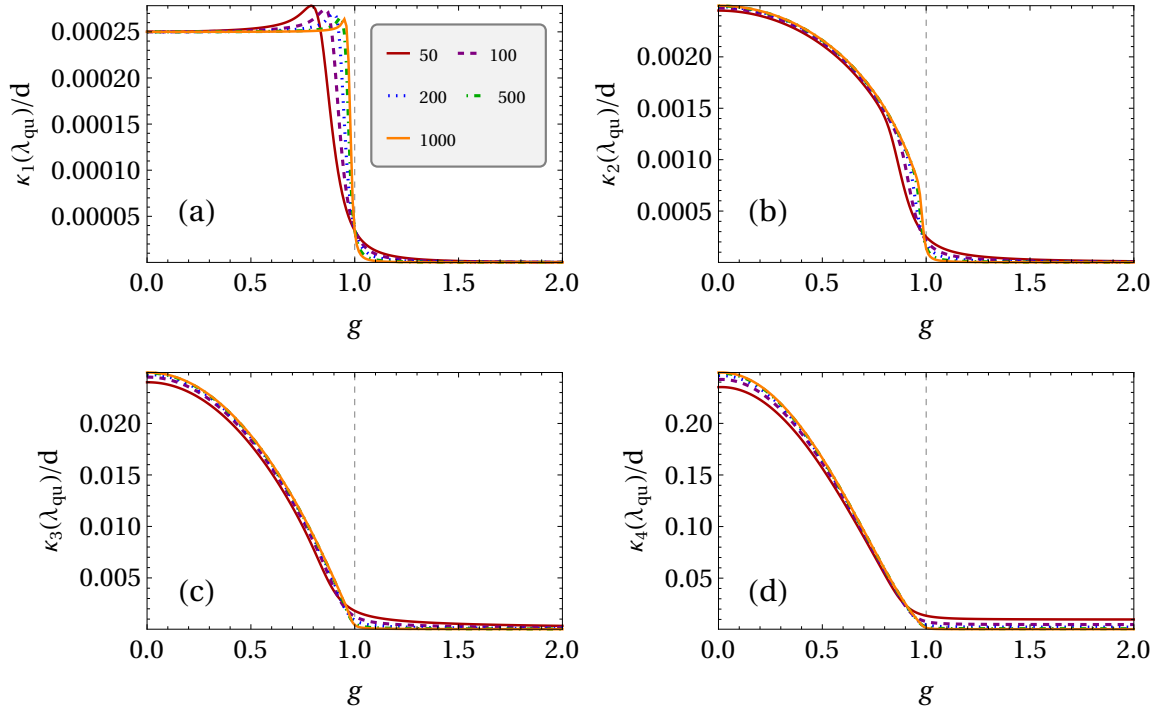
Figure 6.6: Cumulants of λ_{qu} as a function of g for different values of d (LMG model). Other parameters are fixed: $\beta = 10$ and $\delta g = 0.01$.
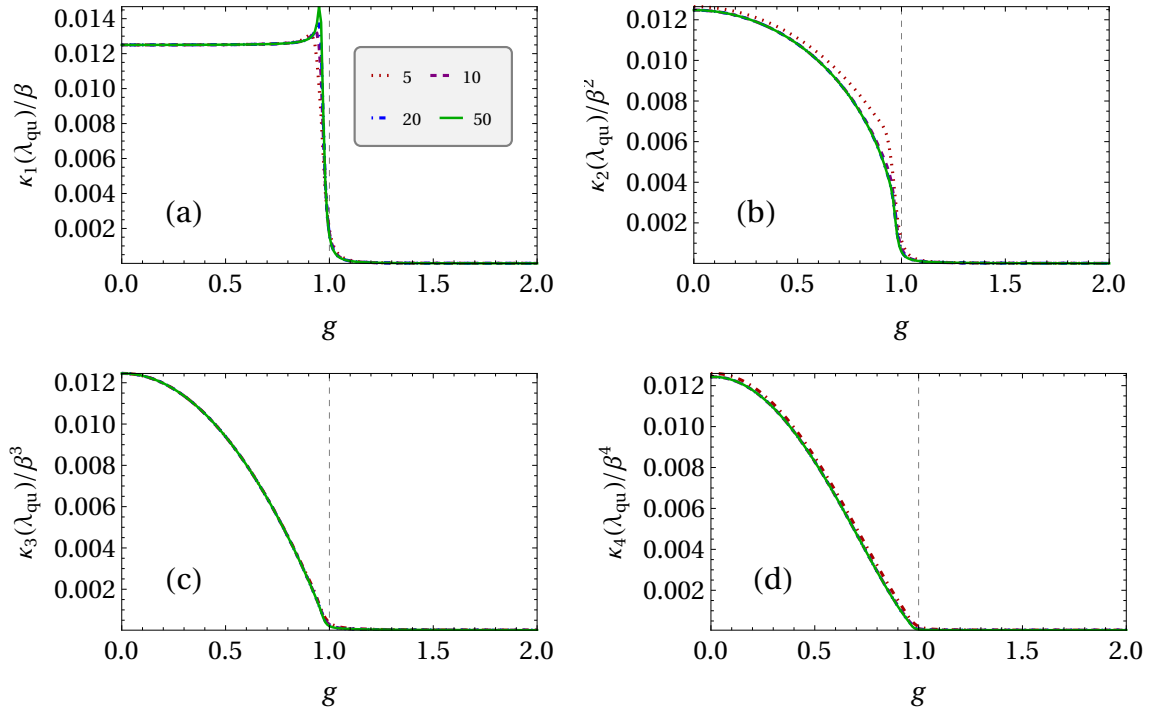
Figure 6.7: Cumulants of λ_{qu} as a function of g for different values of β (LMG model). Other parameters are fixed: $d = 500$ and $\delta g = 0.01$.

Chapter 7

Conclusion

In this dissertation, we studied the statistics of entropy production in work protocols and how coherence contributes to it. We first introduced, in Chapters 2 and 3, the theoretical framework of quantum mechanics and quantum thermodynamics to help understand entropy production and work protocols in the quantum realm. We exposed the formalism for studying the processes in a statistical perspective, and solved the expression for the stochastic entropy production in some limiting cases.

Then, in Chapter 4, we presented the models to which we would apply our propositions: a macrospin system and the Lipkin-Meshkov-Glick (LMG) model. For the first, we solved the model analytically for 1 qubit; for the second, we exposed how the phase transition emerges in the thermodynamic limit (as the dimension tends to infinity). Afterwards, we showed some numerical results for both. In the macrospin, we concluded that, in the thermodynamic limit, the statistics of the entropy production became Gaussian. Also, that it could be achieved for finite dimension, depending on the other parameters of the system: temperature, time of evolution and magnitude of the transverse magnetic pulse. For the LMG model, things worked a bit differently: even for extremely large dimensions and for different values of temperature, we could not observe a Gaussian behavior. Apart from that, the dependence of the cumulants of the distribution with the dimension and the temperature was the same in both models: linear with d and proportional to β^n for the n-th cumulant.

In Chapter 5, we exposed the first proposition of how entropy production could be separated into coherent and diagonal contributions (or quantum and classical), by comparing the final state with its diagonal version in the final energy eigenbasis. We presented analytical results for the first cumulants of the distribution and the form of the cumulant generating function; more in

depth calculations were shown for the limiting cases presented in the previous chapter. We also proposed a backwards process that yields a fluctuation theorem for the stochastic coherence. Contrary to what we would expect [60], we do not have the coherent contribution going to zero in the thermodynamic limit, which we relate to the fact that we have infinite resolution of the energy levels [5]. Also, the dependence of the distribution of γ_{qu} with the parameters is different than that of σ. For the macrospin model, the cumulants tend to saturate for small temperature and large dimension (except for the average Γ_{qu}, that seems to grow logarithmically with d). For the LMG model, the dependence with β is similar to that of the macrospin, but the dependence with the dimension is not, as it appears that the average grows faster than logarithmically and that the variance does not saturate.

In Chapter 6, we presented the second possible splitting of the entropy production, which separates the protocol not considering the final state dephased in the final energy eigenbasis, but the final Hamiltonian dephased in the basis of the final state. We showed some numerical results in order to compare the stochastic behavior of the coherent part with the ones found for the first splitting. We found that the statistics of λ_{qu} was very similar to that of σ. Its dependence with the parameters was the same as the one observed in Chapter 4 for the total entropy production. Also, as happens for γ_{qu}, the average of λ_{qu} does not vanish with increasing dimension, due to the same fine-graining argument.

We do not intend on choosing any splitting as the best one, as both have merits and shortcomings depending on what is being studied [5]. Some future work could be conducted in order to see if there are other useful and meaningful ways of splitting the entropy production into quantum and classical contributions. Other possible future research could investigate what would happen to the statistics of the coherence if we instead considered a coarse graining model. Another interesting topic to be considered for future work is studying deeply the statistics of the entropy production in the LMG model. It was not clear to us why the probability distribution did not behave as a Gaussian, as it did for the macrospin model.

Moreover, the study of coherence at the level of quantum trajectories is relatively new and should still be vastly explored.

Appendix A

Expression for entropy production for thermal operations

Let us consider that the evolution of the composite system ρ_{SE} has a global fixed point, such that

$$U(\bar{\rho}_S \otimes \rho_E)U^\dagger = \bar{\rho}_S \otimes \rho_E. \tag{A.1}$$

We start by taking the logarithm of both sides of the equation. The left-hand side (LHS) gives

$$\log\left[U(\bar{\rho}_S \otimes \rho_E)U^\dagger\right] = U\log(\bar{\rho}_S \otimes \rho_E)U^\dagger$$

$$= U(\log\bar{\rho}_S + \log\rho_E)U^\dagger$$

$$= U\log\bar{\rho}_S\, U^\dagger + U\log\rho_E\, U^\dagger. \tag{A.2}$$

Following the same steps, the right-hand side (RHS) results in

$$\log(\bar{\rho}_S \otimes \rho_E) = \log\bar{\rho}_S + \log\rho_E. \tag{A.3}$$

Therefore, putting both together and operating on both sides with $U^\dagger(\bullet)U$, we get

$$\log\rho_E - U^\dagger\log\rho_E\, U = U^\dagger\log\bar{\rho}_S\, U - \log\bar{\rho}_S. \tag{A.4}$$

Now we recover the expression for the entropy production given in Eq. 3.9,

$$\Sigma = \Delta S_S + \mathrm{tr}\{(\rho_E - \rho'_E)\log\rho_E\}. \tag{A.5}$$

The second term can be rewritten as a trace in both S and E,

$$\mathrm{tr}\{(\rho_E - \rho_E')\log\rho_E\} = \mathrm{tr}_{SE}\{(\rho_S \otimes \rho_E - \rho_{SE}')\log\rho_E\}$$

$$= \mathrm{tr}_{SE}\{(\rho_S \otimes \rho_E)\log\rho_E - U(\rho_S \otimes \rho_E)U^\dagger \log\rho_E\}$$

$$= \mathrm{tr}_{SE}\{(\rho_S \otimes \rho_E)(\log\rho_E - U^\dagger \log\rho_E\, U)\}. \tag{A.6}$$

We recognize the expression above as the LHS of Eq. (A.4), and therefore we can substitute it by the RHS, resulting in

$$\mathrm{tr}\{(\rho_E - \rho_E')\log\rho_E\} = \mathrm{tr}_{SE}\{(\rho_S \otimes \rho_E)(U^\dagger \log\bar{\rho}_S\, U - \log\bar{\rho}_S)\}$$

$$= \mathrm{tr}_{SE}\{(\rho_{SE}' - \rho_S \otimes \rho_E)\log\bar{\rho}_S\}$$

$$= \mathrm{tr}\{(\rho_S' - \rho_S)\log\bar{\rho}_S\}. \tag{A.7}$$

Plugging this result back in Eq. (A.5), we get

$$\Sigma = \Delta S_S + \mathrm{tr}\{(\rho_S' - \rho_S)\log\bar{\rho}_S\}$$

$$= \mathrm{tr}\{\rho_S \log\rho_S\} - \mathrm{tr}\{\rho_S' \log\rho_S'\} + \mathrm{tr}\{\rho_S' \log\bar{\rho}_S\} - \mathrm{tr}\{\rho_S \log\bar{\rho}_S\}$$

$$= S(\rho_S||\bar{\rho}_S) - S(\rho_S'||\bar{\rho}_S). \tag{A.8}$$

Lastly, we recover the fact that the environment is thermal and that thermal operations require energy conservation, i.e., $[U, H_S + H_E] = 0$. As indicated in Ref. [50], the state $\bar{\rho}_S$ that provides a global fixed point is the thermal state ρ_S^{th}, because then $\bar{\rho}_S \otimes \rho_E \propto e^{-\beta(H_S + H_E)}$ and

$$U e^{-\beta(H_S + H_E)} U^\dagger = e^{-\beta(H_S + H_E)}. \tag{A.9}$$

Therefore, the expression for the entropy production for thermal operations is given by

$$\Sigma = S(\rho_S||\rho_S^{th}) - S(\rho_S'||\rho_S^{th}). \tag{A.10}$$

Appendix B

Jarzynski's equalities for γ_{qu} and γ_{cl}

Let us recall the definitions of γ_{qu} and γ_{cl}:

$$\gamma_{\text{qu}}[n, m'] = \log p_n^i - \log p_{m'}^\tau,$$

$$\gamma_{\text{cl}}[n, m'] = \log p_{m'}^\tau - \log p_{m'}^f. \tag{B.1}$$

For γ_{qu}, we have

$$\left\langle e^{-\gamma_{\text{qu}}} \right\rangle = \sum_{n,m'} p_{m'|n} \, p_n^i \exp\left[\log\left(p_{m'}^\tau / p_n^i\right)\right]$$

$$= \sum_{n,m'} p_{m'|n} \, p_{m'}^\tau$$

$$= \sum_{m'} \langle m'| \, U \left\{ \sum_n |n\rangle\langle n| \right\} U^\dagger \, |m'\rangle \, p_{m'}^\tau$$

$$= \sum_{m'} p_{m'}^\tau = 1. \tag{B.2}$$

Lastly, the expression for γ_{cl} is

$$
\begin{aligned}
\left\langle e^{-\gamma_{\mathrm{cl}}} \right\rangle &= \sum_{n,m'} p_{m'|n} \, p_n^i \exp\left[\log\left(p_{m'}^f / p_{m'}^\tau\right)\right] \\
&= \sum_{n,m'} p_{m'|n} \, p_n^i \frac{p_{m'}^f}{p_{m'}^\tau} \\
&= \sum_{m'} \langle m'| \, U \left\{ \sum_n p_n^i \, |n\rangle\langle n| \right\} U^\dagger \, |m'\rangle \frac{p_{m'}^f}{p_{m'}^\tau} \\
&= \sum_{m'} \langle m'| \, U \rho_i^{th} U^\dagger \, |m'\rangle \frac{p_{m'}^f}{p_{m'}^\tau} \\
&= \sum_{m'} \langle m'| \, \rho_\tau \, |m'\rangle \frac{p_{m'}^f}{p_{m'}^\tau} \\
&= \sum_{m'} p_{m'}^f = 1.
\end{aligned}
\tag{B.3}
$$

Appendix C

Other cumulants of γ_{qu} and cumulant generating function

We have already written an expression for the average value of the stochastic coherence, Γ_{qu}. It is interesting to write as well the expression for the variance, $\mathrm{Var}(\gamma_{\mathrm{qu}}) = \langle \gamma_{\mathrm{qu}}^2 \rangle - \langle \gamma_{\mathrm{qu}} \rangle^2$. To do that, we follow the same steps as we used before to compute $\mathrm{Var}(\sigma)$ (Sec. 3.2.3). The first term is given by

$$
\begin{aligned}
\langle \gamma_{\mathrm{qu}}^2 \rangle &= \sum_{n,m'} P[n,m'] \, \gamma_{\mathrm{qu}}[n,m']^2 \\
&= \sum_{n,m'} p_{m'|n} \, p_n^i \left(\log p_n^i - \log p_{m'}^\tau \right)^2 \\
&= \sum_{n,m'} p_{m'|n} \, p_n^i \left[(\log p_n^i)^2 + (\log p_{m'}^\tau)^2 - 2 \log p_n^i \log p_{m'}^\tau \right] \\
&= \sum_{n,m'} p_{m'|n} \, p_n^i (\log p_n^i)^2 + \sum_{n,m'} p_{m'|n} \, p_n^i (\log p_{m'}^\tau)^2 - 2 \sum_{n,m'} p_{m'|n} \, p_n^i \log p_n^i \log p_{m'}^\tau.
\end{aligned}
$$

$$(C.1)$$

Summing the first term in m' and the second in n, we obtain

$$
\langle \gamma_{\mathrm{qu}}^2 \rangle = \sum_n p_n^i (\log p_n^i)^2 + \sum_{m'} p_{m'}^\tau (\log p_{m'}^\tau)^2 - 2 \sum_{n,m'} p_{m'|n} \, p_n^i \log p_n^i \log p_{m'}^\tau. \qquad (C.2)
$$

The first two terms are trivially written in terms of density operators, and for the last term we

carry on with the same strategy used for $\text{Var}(\sigma)$. Therefore, we have that

$$\langle \gamma_{\mathrm{qu}}^2 \rangle = \mathrm{tr}\left\{ \rho_i^{th}(\log \rho_i^{th})^2 \right\} + \mathrm{tr}\left\{ \Delta_f[\rho_\tau](\log \Delta_f[\rho_\tau])^2 \right\} - 2\,\mathrm{tr}\left\{ \log(\Delta_f[\rho_\tau])\,\rho_\tau \log \rho_\tau \right\},$$

(C.3)

and

$$\langle \gamma_{\mathrm{qu}} \rangle^2 = \left(\mathrm{tr}\left\{ \rho_i^{th} \log \rho_i^{th} \right\} - \mathrm{tr}\left\{ \Delta_f[\rho_\tau] \log \Delta_f[\rho_\tau] \right\} \right)^2, \tag{C.4}$$

so the variance is given by $\text{Var}(\gamma_{\mathrm{qu}}) = \langle \gamma_{\mathrm{qu}}^2 \rangle - \langle \gamma_{\mathrm{qu}} \rangle^2$, with $\langle \gamma_{\mathrm{qu}}^2 \rangle$ and $\langle \gamma_{\mathrm{qu}} \rangle^2$ given by Eqs. (C.3) and (C.4).

Another interesting quantity to compute is the *cumulant generating function* (CGF) of γ_{qu}. It is defined as

$$K_{\gamma_{\mathrm{qu}}}(\lambda) := \log \left\langle e^{-\lambda \gamma_{\mathrm{qu}}} \right\rangle, \tag{C.5}$$

where $\lambda \in \mathbb{C}$. If we substitute the expression for γ_{qu}, we obtain

$$K_{\gamma_{\mathrm{qu}}}(\lambda) = \log \left\{ \sum_{n,m'} p_{m'|n}\, p_n^i \exp\left[-\lambda \log\left(p_n^i / p_{m'}^\tau \right) \right] \right\}$$

$$= \log \left[\sum_{n,m'} p_{m'|n}\, p_n^i \left(\frac{p_{m'}^\tau}{p_n^i} \right)^\lambda \right]. \tag{C.6}$$

Inspired by Reference [4], let us rewrite the CGF in terms of traces. Proceeding from Eq. (C.6), we have that

$$K_{\gamma_{\mathrm{qu}}}(\lambda) = \log \left[\sum_{n,m'} p_{m'|n}\, p_n^i \left(\frac{p_{m'}^\tau}{p_n^i} \right)^\lambda \right]$$

$$= \log \left[\sum_{n,m'} (p_{m'}^\tau)^\lambda (p_n^i)^{1-\lambda} |\langle m'|U|n \rangle|^2 \right]$$

$$= \log \left\{ \sum_{m'} \langle m|' \Delta_f[\rho_\tau]^\lambda\, U \left[\sum_n (p_n^i)^{1-\lambda} |n\rangle\langle n| \right] U^\dagger |m'\rangle \right\}$$

$$= \log \left\{ \mathrm{tr}\left[\Delta_f[\rho_\tau]^\lambda\, U\, (\rho_i^{th})^{1-\lambda}\, U^\dagger \right] \right\}. \tag{C.7}$$

Finally, by applying the unitaries to the initial state ρ_i^{th}, we obtain

$$K_{\gamma_{\mathrm{qu}}}(\lambda) = (\lambda - 1)\, S_\lambda(\Delta_f[\rho_\tau]||\rho_\tau), \tag{C.8}$$

where we used the definition of the λ-Rényi divergence,

$$S_\lambda(\rho||\sigma) := \frac{1}{\lambda - 1} \log \operatorname{tr}\left[\rho^\lambda \sigma^{1-\lambda}\right]. \tag{C.9}$$

The cumulants are obtained by differentiating the CGF, i.e.,

$$\kappa_n(\gamma_{qu}) := (-1)^{-n} \left.\frac{\mathrm{d}^n K_{\gamma_{qu}}(\lambda)}{\mathrm{d}\lambda^n}\right|_{\lambda=0}. \tag{C.10}$$

Appendix D

Comparison between limiting cases for a qubit using the macrospin model

For the first case, we consider $H_i = H_f = -h_z S_z$, $H = -h_z S_z - h_x S_x$, $\tau \ll 1$. The average Γ_{qu} is given by

$$\Gamma_{\text{qu}}^{(1)} = \tau^2 \sum_{n,m'} p_n^i \log p_n^i / p_m^i \, | \langle m | H | n \rangle |^2. \tag{D.1}$$

Now, for the second limit case, $H_i = -h_z S_z$, $H_f = H_i + \delta H$, with $\delta H = -h_x S_x \ll H_i$. The expression for the average of γ_{qu} is

$$\Gamma_{\text{qu}}^{(2)} = \sum_n \sum_{m \neq n} p_n^i \log p_n^i / p_m^i \, \frac{| \langle m | \delta H | n \rangle |^2}{(\epsilon_m - \epsilon_n)^2}. \tag{D.2}$$

In the first case, we see that the only terms left will be the ones for $m \neq n$, because $\log p_n^i / p_n^i = \log 1 = 0$. So

$$| \langle m | H | n \rangle |^2 = | -h_x/2 |^2 = \frac{h_x^2}{4}, \quad \text{for } m \neq n, \tag{D.3}$$

which is the exactly same result we obtain for $| \langle m | \delta H | n \rangle |^2$. Now, we solve for

$$\tau^2 \sum_n \sum_{m \neq n} p_n^i \log p_n^i / p_m^i = \sum_n \sum_{m \neq n} p_n^i \log p_n^i / p_m^i \, (\epsilon_m - \epsilon_n)^{-2}. \tag{D.4}$$

Since we are dealing with a qubit, the difference between energies squared is constant and equal

to $(\epsilon_1 - \epsilon_2)^2 = h_z^2$. So, finally, we conclude that

$$\tau = h_z^{-1}, \tag{D.5}$$

where τ and h_z are always non-negative. The same will happen for all the cumulants $\kappa_j(\gamma_{\text{qu}})$, and therefore we conclude that the distributions are identical in this case, meaning that the entropy production due to coherence fluctuations is the same.

Appendix E

Jarzynski's equalities for λ_qu and λ_cl

Given the definitions

$$\lambda_\mathrm{qu}[n, m'] := \log \tilde{p}_n^f - \log p_{m'}^f, \tag{E.1}$$

$$\lambda_\mathrm{cl}[n, m'] := \log p_n^i - \log \tilde{p}_n^f, \tag{E.2}$$

the Jarzynski equality for λ_cl becomes

$$\begin{aligned}
\left\langle e^{-\lambda_\mathrm{cl}} \right\rangle &= \sum_{n,m'} p_{m'|n} \, p_n^i \exp\left[\log\left(\tilde{p}_n^f / p_n^i\right)\right] \\
&= \sum_{n,m'} p_{m'|n} \, \tilde{p}_n^f \\
&= \sum_n \langle n| \, U^\dagger \left\{ \sum_{m'} |m'\rangle\langle m'| \right\} U \, |n\rangle \, \tilde{p}_n^f \\
&= \sum_n \tilde{p}_n^f = 1.
\end{aligned} \tag{E.3}$$

However, for λ_{qu}, it is given by

$$
\begin{aligned}
\left\langle e^{-\lambda_{\text{qu}}} \right\rangle &= \sum_{n,m'} p_{m'|n}\, p_n^i \exp\left[\log\left(p_{m'}^f / \tilde{p}_n^f\right)\right] \\
&= \sum_{n,m'} p_{m'|n}\, p_n^i \frac{p_{m'}^f}{\tilde{p}_n^f} \\
&= \sum_n \langle n|\, U^\dagger \left\{ \sum_{m'} p_{m'}^f\, |m'\rangle\langle m'| \right\} U\, |n\rangle \frac{p_n^i}{\tilde{p}_n^f} \\
&= \sum_n \langle n|\, U^\dagger \rho_f^{th} U\, |n\rangle \frac{p_n^i}{\tilde{p}_n^f} \\
&= \operatorname{tr}\{ U^\dagger \rho_f^{th} (\tilde{\rho}_f^{th})^{-1} U \rho_i^{th} \} \\
&= \operatorname{tr}\{ \rho_f^{th} (\tilde{\rho}_f^{th})^{-1} \rho_\tau \}.
\end{aligned}
\tag{E.4}
$$

This expression cannot be further simplified. Then, λ_{qu} does not satisfy a fluctuation theorem.

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