Universidade de São Paulo
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Modelos colisionais: ambientes e termodinâmica

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Orientador: Prof. Dr. Gabriel Teixeira Landi.

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University of São Paulo
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Collisional models: thermodynamics and reservoirs

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Supervisor: Prof. Dr. Gabriel Teixeira Landi.

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Primeiro levaram os negros
Mas não me importei com isso
Eu não era negro
Em seguida levaram alguns operários
Mas não me importei com isso
Eu também não era operário
Depois prenderam os miseráveis
Mas não me importei com isso
Porque eu não sou miserável
Depois agarraram uns desempregados
Mas como tenho meu emprego
Também não me importei
Agora estão me levando
Mas já é tarde.
Como eu não me importei com ninguém
Ninguém se importa comigo.
— Intertexto, Bertold Brecht.

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Abstract

The physical modelling of reservoirs is a very hard problem given the uncountable number of particles that it is composed of. In the thermal case, we can resort to the laws of thermodynamics. The problem changes completelly when it is not possible to assume that the reservoir is at thermal equilibrium. Not only one does not have memory enough to encode all of its degrees of freedom, as one also cannot access each degree individually. Thus, to describe the effect such reservoir induces on a system of interest, several approximations are needed, as weak coupling between system and environment, which is supposed to be composed of independent thermalized particles. To deal with these restrictions, we use the collisional model. It is an intuitive framework that has guaranteed control over all its degrees of freedom, as one can freely choose the initial state of its constituents.

In this work, we expose the results in the literature that extract thermodynamics out of the collisional model when the particles that compose it are in a thermal state. Inspired by this result, we show that a special class of non-equilibrium states exists such that thermodynamics can also be drawn from them. This class posses a small amount of coherence in them, and through our model we can connect the dynamics of this coherence in the reservoir with the energy it transfers to the system connected to it, paving the way to a long desired bridge between quantum and classical resources.

Keywords: thermodynamics, coherence, open systems, quantum information, resource theory.

Resumo

A modelagem física de um reservatório é um problema extremamente difícil dado o incontável número de partículas que o compõe. No caso térmico, podemos recorrer às leis da termodinâmica. O problema toma outra forma quando é inviável assumir que o ambiente se encontra em equilíbrio térmico. Além de não termos memória suficiente para gravar todos os seus graus de liberdade, não temos controle experimental suficiente para acessar cada um deles individualmente. Portanto, para descrever o efeito que tal reservatório induz em um sistema de interesse, precisamos de diversas aproximações e hipóteses, como acoplamento fraco entre sistema e reservatório, que por sua vez supõe-se ser constituído de partículas independentes inicializadas num estado térmico. Para lidar com estas restrições, usamos neste trabalho o modelo colisional —um modelo de ambiente intuitivo que garante controle de seus graus de liberdade, do qual escolhe-se o estado inicial de seus constituintes.

Nesse trabalho, expomos os resultados da literatura de que a termodinâmica pode ser extraída do modelo colisional quando as partículas que compõe o ambiente são térmicas. Enfim, mostramos que existe uma classe especial de sistemas fora do equilíbrio térmico que também respeitam as leis da termodinâmica. Os estados dessa classe possuem uma pequena quantidade de coerência, e por meio do nosso modelo fazemos uma conexão entre a dinâmica da coerência do ambiente e a troca de energia que ele realiza com o sistema. Esse estudo, portanto, abre portas para a tão desejada conexão entre recursos quânticos e clássicos.

Palavras-chave: termodinâmica, coerência, sistemas abertos, informação quântica, teoria de recursos.

List of Figures

Contents

Chapter 1

Introduction

Thermodynamics arose in the context of the industrial revolution, where an operational set of laws where needed to better describe the behavior of heat engines and refrigerators. The first law states energy conservation, by separating the energy of the accessible degrees of freedom (work) and the inaccessible ones (heat); the second law sets a limit on the best-case scenario work output of an engine. The success of this framework mostly resides on the clear description it offers for an astonishingly broad applicability. Although the second law provides bounds for arbitrary processes, only a restrict set of transformations, named quasi-equilibrium processes, enjoys their saturation [1]. Thus the precise mechanisms underlying non-equlibrium transformations are not clear: it is only possible to infer that they are lower bounded by the quasi-equilibrium ones.

The reemergence of the atomism view in the end of the nineteenth century rendered the axiomatic theory of thermodynamics obsolete, left to be defended only by those influenced by the positivism movement. The atomists rewrote thermodynamics as a mechanical theory, such as the kinetic theory of gases, putting it as a microscopic theory rather than an operational one. This resulted in the formulation of statistical mechanics, which shed new light onto the meaning of heat and temperature: they were thought as a statistical average over the trajectories of a large number of particles. At the expense of a justifying connection with classical mechanics, thermodynamics became a theory defined only for a macroscopic number of particles [2].

These results hold for classical trajectories, all derived before the advent of quantum mechanics. It was not until the end of XX century that research on thermodynamics pointed towards a conciliation of its concepts with quantum physics. To enlist a few reasons of why was that so, one could say that it would not make sense to apply a theory most relevant in the microworld to a theory of the macroworld; One could also argue that thermodynamics is ultimately operational, and no operational machine used quantum mechanical concepts such as entanglement or coherence in a clear manner at the time. The actual interest in developing a theory that would define heat and work for quantum mechanics came when thermodynamics was defined for systems of arbitrary size through stochastic thermodynamics [3], due to the connection of information erasure and heat dissipation as done by Landauer [4], and when it was shown that a genuine quantum property, such as entanglement, turned possible some computational protocols that were believed to be impossible, such as prime factorization in polinomial time [5].

In this sense, a quantum quantity such as entanglement was put on an equal footing with a thermodyncamical quantity such as work: both are resources to be utilized for a given task. They are all studied under the formalism of resource theories [6], where structural connections where made both theoretically [7–9] and experimentally [10, 11].

But is there a direct bridge between quantum features and the usual thermodynamical setting of engines and refrigerators? Research was already done in this direction with entanglement [12] and coherence [13], but the only scenario where there is a reformulation of the laws of thermodyncamics is in the case of squeezing [14, 15].

The objective of this work is to understand whether such reformulation can be done with coherence. To deal with this problem, we need a way to deal with general reservoirs that are not necessarily thermal, as thermal states yield no coherence.

A framework for studying reservoirs that has draw attention in the last decade for its outstanding balance of simplicity and versatility is the collisional model [16–29]. It depicts the contact with the environment as a sequence of two body interactions between the system of interest and particles of an ensemble, leading to a description in terms of successive maps. If the coupling is made weak enough, an effective differential equation can be written for some energy scales. In particular, if the ensemble is made of thermal states, a master equation identical to that of thermal baths is derived. In this scenerio, the discrete map is dubbed thermal operation [30, 31] and thermodynamics can be drawn from it [21].

We inspire in this result to study the case in which the particles the system collides with are in a thermal state with a small amount of coherences. This out of equilibrium states also provide a master equation description, where the coherences give rise to a Hamiltonian contribution. Moreover, it is shown that the thermodynamic laws not only are still valid in this regime, as they earn an additional structure concerning the environment's coherence change rate. This is made in connection with the second law, where the the change in the relative entropy of coherence set a tighter bound on work extraction than the free energy difference [32].

The ouline of the dissertation goes as follows: in Chapter 2 the formalism of quantum information are briefly developed to introduce the reader to key concepts to be used throughout the text. In Chapter 3, we present the formalism of quantum operations, which are an extention of the unitary evolution that one would learn in a standard course on quantum mechanics. This extension is needed whenever the system of interest is composite, a crucial property of a system to be opened to an environment. Using this framework, we combine it with information-theoretic tools to construct a way to quantify coherence in Chapter 4. Chapter 5 devotes to a special type of quantum operation: the master equation. It is a differential equation for a system in contact with an environment that is widely used to model large reservoirs. Finnaly, in Chapter 6, the collisional model is presented alongside the novel results proposed by the author and his collaborators. In the end we offer a conclusion for the presented material.

From now on, every statement is done for finite dimentional Hilbert spaces in the context of quantum theory: no allusion to classical mechanics is done unless specified.

Chapter 2

Quantum information

Entropy is a key concept in physics. From the perspective of thermodynamics, it is central to the notion of irreversibility and the emergence of the so called thermodynamic arrow of time, as irreversible processes must be acompanied by an entropy increase [33]. However, in probability theory, it serves as a measure of randomness and disorder of a sample space through its probability distribution [34]. As these concepts are hard to conciliate, an independent meaning of entropy becomes elusive. However, the advent of statistical mechanics gave insight on the connection between irreversibility and disorder [35]. Half a century ago, a new perception of the meaning of entropy reopened the discusion on the connections entropy provides. This took place on the development of information theory in the 1950s, where Claude Shannon proved the noiseless coding theorem: the entropy of a probability distribution of certain events in a message sets the limit for the message compression [36]. As the message cannot be compressed further, its string length is defined as its information content. In the following sections, this definition of information will be revisited in the quantum scenario, as later on the dissertation it will be connected with thermodynamics.

2.1 Entropy as an information measure

It was stated that the Shannon entropy H of a distribution p is a measure of information. It is written as [36]

$$H(p) = \sum_{n=1}^{d} p_n \log_2 p_n, \tag{2.1}$$

where the distribution is assumed to be discrete over d possible outcomes and the logarithm is taken on base 2, for the entropy/information is measured in bits. Now, for a general quantum system ρ, the entropy chosen is the von Neumann entropy $S(\rho)$:

$$S(\rho) = -\mathrm{Tr}\{\rho \log \rho\}. \tag{2.2}$$

It is defined this way so that it matches the classical case when the state is a classical distribution of its eigenstates: [37]

$$\begin{aligned} S(\rho) = -\mathrm{Tr}\{\rho \log \rho\} &= -\sum_{\mathrm{n}} \langle \mathrm{n}| \rho \log \rho |\mathrm{n}\rangle \\ &= -\sum_{n} p_n \log p_n, \end{aligned} \tag{2.3}$$

where $\rho |n\rangle = p_n |n\rangle$. The only difference is that here the natural logarithm is taken, for simplicity.

Although Shannon's theorem gives entropy an operational meaning, viz. data compression, whilst defining information, there is not a single interpretation on how entropy relates to information. One of them considers that entropy measures the lack of information an observer has about the system before measuring it. The other considers that entropy measures the amount of information obtained after one measures the quantum state. Hence, one can regard entropy both as information or the lack of it, depending on whether one puts oneself before or after the action of measurement [38]. Both views are complementary and do not interfere with one another, thus the most convenient view will be adopted for each case at hand.

For instance, a pure state $|\psi\rangle \langle\psi|$ is itself an eigenstate with probability 1, and thus the entropy is 0. This copes well with intuition, since a pure state lacks no information: with a pure state one knows everything there was to know about it. On the other hand, once one measures a pure state, no new information is gained, as the state of the system as already known. Notice that it is considered here that one can measure in the right basis as to obtain a deterministic result.

As a complementary example, consider the maximally mixed state ρ_{mix}. By definition, the only information it contains is the dimension d of its Hilbert state. The von Neumann entropy reflects well this notion:

$$S(\rho_{mix}) = -\sum_{n=1}^{d} p_n \log p_n = -\sum_{n=1}^{d} \frac{1}{d} \log \frac{1}{d} = \log d. \tag{2.4}$$

Here, all p_n are equal to $1/d$, as a consequence of the number of possible equiprobable measurement outcomes. As expected, the entropy in this case is non-zero, for the maximally mixed state contains no information about which state the system is in, and again, returns a finite amount of information once measured.

An important consequence of the unitarity of quantum mechanics is that entropy is conserved:

$$S(\rho_t) = S(U\rho U^\dagger) = US(\rho)U^\dagger = S(\rho), \tag{2.5}$$

where U is any unitary operator. In the last equality the property of unitaries to freely get inside and outside the argument of analytical functions was used. Although trivial, the conservation of entropy in quantum theory is a major departure from classical information theory.

The von Neumann entropy is additive for product states. For instance, if $\rho_{AB} = \rho_A \otimes \rho_B$, then

$$S(\rho_{AB}) = S(\rho_A) + S(\rho_B). \tag{2.6}$$

This means that the information of the joint system is the sum of the information of its parts. It is an intuitive property if one notices that in a product state there is no connection between the parts, and hence the information in one of them cannot interfere with the information of the other one. Yet not always the state that lives in the joint Hilbert space of A and B can be cast as a product state of both spaces. To better understand what happens in the latter case, it is useful to develop the concept of relative entropy. Subsection 2.1.1 gives a brief description of the relative entropy, and subsection 2.1.2 uses it to address the posed problem.

2.1.1 Relative entropy

A useful tool for deriving relations and building intuition on information theory is the relative entropy, or Kullback-Leibler divergence [39]. The definition goes as follows:

$$S(\rho\|\sigma) = \mathrm{Tr}\{\rho\log\rho\} - \mathrm{Tr}\{\rho\log\sigma\}. \tag{2.7}$$

The main reason for using it is that it offers a non-trivial inequality regarding two different quantum states, the Klein's inequality [38]:

$$S(\rho\|\sigma) \geq 0, \tag{2.8}$$

$$S(\rho\|\sigma) = 0 \text{ iff } \rho = \sigma. \tag{2.9}$$

The proof is out of the scope of this work. Several results can be derived from it, for instance the information gained by measuring a maximally mixed state is the highest possible in a given dimension:

$$\begin{aligned} S(\rho\|\rho_{mix}) &= \mathrm{Tr}\{\rho\log\rho\} - \mathrm{Tr}\{\rho\log\rho_{\mathrm{mix}}\} = -\mathrm{S}(\rho) - \sum_{\mathrm{n=1}}^{\mathrm{d}} \langle \mathrm{n}|\,\rho\log(\mathbb{I}/\mathrm{d})\,|\mathrm{n}\rangle \\ &= -S(\rho) + \log d\ \mathrm{Tr}\rho = -\mathrm{S}(\rho) + \log \mathrm{d} \geq 0 \end{aligned}$$

where $\mathbb{I}$ is the identity matrix and $\mathrm{Tr}\rho = 1$ is just the normalization of density matrix. As imagined, the state that returns the highest amount of information after a measurement is the maximaly mixed state:

$$S(\rho) \leq \log d. \tag{2.10}$$

It is important to make a small digression before delving into further applications. Eq. (2.8) tempts one to regard Eq. (2.7) as a distance between density matrices. However, that is not the case. One way to see this is by noting that the relative entropy is not symmetrical. For instance, consider the density matrices

$$\rho_A = \begin{pmatrix} 0.2 & 0 \\ 0 & 0.8 \end{pmatrix}, \qquad \rho_B = \begin{pmatrix} 0.3 & 0 \\ 0 & 0.7 \end{pmatrix},$$

then their relative entropies read

$$\begin{aligned} S(\rho_A\|\rho_B) &= 0.2\log 0.2 + 0.8\log 0.8 - 0.2\log 0.3 - 0.8\log 0.7 = 0.026, \\ S(\rho_B\|\rho_A) &= 0.3\log 0.3 + 0.7\log 0.7 - 0.3\log 0.2 - 0.7\log 0.8 = 0.028. \end{aligned}$$

Furthermore, the relative entropy will not generally respect the triangle inequality $S(\rho\|\sigma) \leq S(\rho\|\tau) + S(\tau\|\sigma)$.

2.1.2 Subadditivity and mutual information

The relative entropy, in particular the Klein inequality, allows a thorough discussion of the question raised: how does the entropy of a composite quantum system living in $\mathbb{H} = \mathbb{H}_A \otimes \mathbb{H}_B$ relate to the entropy of its parts when the system is not a product state? To answer this, consider the relative entropy between the state ρ_{AB} and $\rho_A \otimes \rho_B$, where $\rho_A = \mathrm{Tr_B}\rho_{\mathrm{AB}}$, $\rho_B = \mathrm{Tr_A}\rho_{\mathrm{AB}}$ and $\mathrm{Tr_X}$ is the partial trace with respect to Hilbert space $\mathbb{H}_X$:

$$S(\rho_{AB} \| \, \rho_A \otimes \rho_B) = -S(\rho_{AB}) - \mathrm{Tr}\{\rho_{\mathrm{AB}} \log(\rho_{\mathrm{A}} \otimes \rho_{\mathrm{B}})\} \tag{2.11}$$

Using Eq. (2.8) and $\log(\rho_A \otimes \rho_B) = \log(\rho_A) + \log(\rho_B)$,

$$S(\rho_{AB}) \leq -\mathrm{Tr}\{\rho_{\mathrm{AB}} \log \rho_{\mathrm{A}}\} - \mathrm{Tr}\{\rho_{\mathrm{AB}} \log \rho_{\mathrm{B}}\}. \tag{2.12}$$

To proceed, we use the fact that the trace is a concatenation of partial traces:

$$S(\rho_{AB}) \leq -\mathrm{Tr_A}\{\mathrm{Tr_B}\rho_{\mathrm{AB}} \log \rho_{\mathrm{A}}\} - \mathrm{Tr_B}\{\mathrm{Tr_A}\rho_{\mathrm{AB}} \log \rho_{\mathrm{B}}\} \tag{2.13}$$

$$S(\rho_{AB}) \leq -\mathrm{Tr}\{\rho_{\mathrm{A}} \log \rho_{\mathrm{A}}\} - \mathrm{Tr}\{\rho_{\mathrm{B}} \log \rho_{\mathrm{B}}\} \tag{2.14}$$

$$S(\rho_{AB}) \leq S(\rho_A) + S(\rho_B). \tag{2.15}$$

The relation (2.15) is known as the subadditive property of the von Neumann entropy [38]. It states that the entropy of a joint system is upper bounded by the entropy of its parts, and the bound is saturated when the system is already in a product state. In the language of information theory, information about the system is lost if one only looks locally at its parts. This raises the question: where does this information reside? If the information about the composite system is not only the sum of the information about its parts, then where is the rest of it? The usual interpretation is that it resides in the correlations between the local elements of the system, and as such one can only access it by means of global (instead of local) operations.

This motivates the definition of the measure of information stored as correlations between subsystems A and B, the mutual information:

$$\mathcal{I}(A:B) := S(A) + S(B) - S(AB) \geq 0. \tag{2.16}$$

Notice that Eq. (2.8) provides the desired non-negativity of the mutual information, a crucial property of an information measure.

Chapter 3

Quantum operations

The postulates of quantum dynamics impose unitary evolution to systems that are not disturbed by an observer [37]. Thus, given that a system is ininitially in state $|\psi\rangle$, then the only possible final state should be $|\psi'\rangle = U|\psi\rangle$, where U is any unitary transformation. Notice that the purity of the state is conserved through the evolution:

$$\mathcal{P}(|\psi'\rangle\langle\psi'|) = \mathrm{Tr}\{|\psi'\rangle\langle\psi'|\} = \mathrm{Tr}\{\mathrm{U}|\psi\rangle\langle\psi|\mathrm{U}^\dagger\} = \mathrm{Tr}\{\mathrm{U}^\dagger\mathrm{U}|\psi\rangle\langle\psi|\} = \mathrm{Tr}\{|\psi\rangle\langle\psi|\} \tag{3.1}$$

Then one could raise the following question: if unitary operators preserve purity, how does pure states evolve into mixed states? In order to understand how this kind of transformation takes place, this chapter delevelops the concept of quantum operations: a generalization of unitary transformations that allow for a state to dynamically change its purity. For this merit, the formalism of quantum operations is widely used in the open quantum systems community, as a real experiment cannot prevent losses from occuring [38].

Quantum operations have three main representations that reflect its importance in different scenarios. The first one is the operator-sum representation, or Kraus representation [40, 41]. This form often omits the intermediate dynamics of the system, just relating inputs and outputs. It is a strong tool for the quantum information and quantum computation community [38], and will be studied in Section 3.1. The second one, in connection with the theory of open quantum systems, is the Stinespring dilation [42]. It states that every quantum operation can be cast as an unitary evolution in an extension of the original Hilbert space, and will be covered in Section 3.2. The third one is the axiomatic definition or Choi representation, where it is proved from a small set of physically motivated axioms that the most general equation possible is a quantum operation [43,44], and will be covered in Section 3.3.

3.1 Quantum channels and the operator-sum representation

In the Kraus representation, a quantum operation Φ is written as

$$\Phi[\rho] = \sum_i K_i \rho K_i^\dagger, \tag{3.2}$$

$$\sum_i K_i^\dagger K_i = \mathbb{1}, \tag{3.3}$$

where the K_i are positive operators known as Kraus operators. An interpretation of the individual K_i will be provided later on. Before that, let us explore a famous example using this formalism, the dephasing channel Φ_{deph} for a qubit state:

$$K_1 = \sqrt{1-\lambda}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \tag{3.4}$$

$$K_2 = \sqrt{\lambda}\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \tag{3.5}$$

$$K_3 = \sqrt{\lambda}\begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \tag{3.6}$$

where λ is a real parameter ranging from 0 to 1. The effect of the dephasing map on an arbitrary state

$$\rho = \begin{pmatrix} p & q \\ q^* & 1-p \end{pmatrix} \tag{3.7}$$

reads

$$K_1 \rho K_1^\dagger = (1-\lambda)\rho, \tag{3.8}$$

$$K_2 \rho K_2^\dagger = \lambda \begin{pmatrix} p & 0 \\ 0 & 0 \end{pmatrix}, \tag{3.9}$$

$$K_3 \rho K_3^\dagger = \lambda \begin{pmatrix} 0 & 0 \\ 0 & 1-p \end{pmatrix}, \tag{3.10}$$

$$\Phi_{deph}[\rho] = \sum_{i=1}^{3} K_i \rho K_i^\dagger = (1-\lambda)\rho + \lambda \rho_{\text{diag}}, \tag{3.11}$$

where ρ_{diag} is the state ρ without its off-diagonal elements. Thus, the map is a convex combination of the original density matrix and a density matrix that lost its off-diagonal elements, the coherences. This phenomenon is known both as decoherence or dephasing, where the latter designation coins the map's name. This is a phenomenon that forces a quantum system to be diagonal in a basis induced by an environment, as will be seen in Chapter 5. Notice that there is no information on how this decoherence took place: just the initial and final states are of interest, there is no reference to time. In Chapter 5 this map will be derived from first principles in real a physical setup.

This example gives a glance on how to interpret the individual Kraus operators. Considering only the action of K_1 on ρ, one notices it does nothing: it is just a reescaling of the identity: the state is the same up to normalization. Although it will play a role in the discusion, let us overlook the normalization factors for now. The action of K_2 destroys coherences by projecting the state onto the ground state. K_3 does the same, although it projects ρ onto the excited state. This hints that the different Kraus operators provides information on the possible events the quantum state can experience. This interpretation of the operator-sum decomposition is called quantum jumps dynamics, where each Kraus operator is associated with an action on the system, or jump [45]. Here, the possible jumps for the system are projecting onto the ground state, projecting onto the excited state, or nothing happening. The normalization factors are then interpreted as the probability with each jump. This is very used in the light of stochastic processes, as it is similar in structure to a random walk . In this stochastic interpretation, Eq. (3.2) is an average over all possible transformation the state would suffer. This is transformation becomes approximately exact, but for each individual system a single stochastic trajectory should occur. If one follows this trajectory by constantly monitoring the system, then Eq. (3.2) breaks down, and the system would follow individual jumps with no ensemble average:

$$\rho_n = \frac{K_n \rho K_n^\dagger}{p_n}, \tag{3.12}$$

where the normalization factor $p_n = \text{tr}\{K_n \rho K_n^\dagger\}$ is the jump probability. This is refered to as post-selection, as the monitoring allows one to follow a desired trajectory, or dynamics, by discharting the remaining possible outcomes. As stated before, the original formulation for a map Φ is the averaging over the possible density matrices ρ_n:

$$\Phi[\rho] = \sum_n K_n \rho K_n^\dagger = \sum_n p_n \rho_n. \tag{3.13}$$

More will be covered on the operator-sum representation on the following sections, nevertheless we finish this presentation with an important property of this type of map: different Kraus operators may refer to the same dynamics. Take the linear transformation

$$N_i = \sum_j U_{ij} K_j. \tag{3.14}$$

In order for the set of N_i to also be Kraus operators, we must have

$$\sum_i N_i^\dagger N_i = \sum_{j,k} K_j^\dagger K_k \sum_i U_{ij}^* U_{ik} = \mathbb{1}. \tag{3.15}$$

Since the set of operators K_i respect Eq. (3.3), it is sufficient for the N_i to be Kraus operators that U is unitary, such that $\sum_i U_{ij}^* U_{ik} = \delta_{jk}$. This implies that

$$\sum_i N_i \rho N_i^\dagger = \sum_{j,k} K_k \rho K_j^\dagger \sum_i U_{ij}^* U_{ik} = \sum_j K_j \rho K_j^\dagger. \tag{3.16}$$

Thus, if the Kraus operators are all changed by a unitary transformation, the complete map does not change. Although the map is unique, the operator-sum representation is not.

3.2 Environment perspective

For its simplicity, the operator-sum representation is very practical to derive general results for all quantum operations. However, as it was presented, its use seems ad hoc, with no connection with the postulates of quantum dynamics. The connection exists and is very beautiful, though. Consider a closed quantum system $\rho \in \mathbb{H}$ evolving under a unitary U:

$$\rho' = U\rho U^\dagger. \tag{3.17}$$

Now, suppose this quantum system is structured, i.e. composed of $\rho_A \in \mathbb{H}_A$ and $\rho_B \in \mathbb{H}_B$ where $\mathbb{H} = \mathbb{H}_A \otimes \mathbb{H}_B$ and $\rho_{A(B)} = \mathrm{tr}_{B(A)}\,\rho$. Furthermore, assume they are initially uncorrelated, viz. $\rho = \rho_A \otimes \rho_B$. The evolution for ρ_A alone reads

$$\rho'_A = \mathrm{tr}_B\,\rho' = \mathrm{tr}_B\{U(\rho_A \otimes \rho_B)U^\dagger\}. \tag{3.18}$$

Since any operator U living in $\mathbb{H} = \mathbb{H}_A \otimes \mathbb{H}_B$ can be written as [46]

$$U = \sum_i A_i \otimes B_i \quad A(B)_i \in \mathbb{H}_{A(B)}, \tag{3.19}$$

then

$$\rho'_A = \sum_{i,j} \mathrm{tr}_B\{A_i B_i (\rho_A \rho_B) A_j^\dagger B_j^\dagger\} = \sum_{i,j} \mathrm{tr}_B\{A_i \rho_A A_j^\dagger B_i \rho_B B_j^\dagger\} \tag{3.20}$$

$$\rho'_A = \sum_{i,j} A_i \rho_A A_j^\dagger\, \mathrm{tr}\{B_i \rho_B B_j^\dagger\} = \sum_{i,j} \lambda_{ij} A_i \rho_A A_j^\dagger, \tag{3.21}$$

where $\lambda_{ij} := \mathrm{tr}\{B_i \rho_B B_j^\dagger\} = \lambda_{ji}^*$. As the matrix formed by the λ_{ij} is hermitian, we can diagonalize it:

$$\lambda_{ij} = \sum_k m_{ik} \lambda_k m_{jk}^*. \tag{3.22}$$

Inserting in Eq. (3.21),

$$\rho'_A = \sum_k \Big(\sqrt{\lambda_k} \sum_i m_{ik} A_i\Big) \rho_A \Big(\sqrt{\lambda_k} \sum_j m_{kj}^* A_j^\dagger\Big) = \sum_k K_k \rho_A K_k^\dagger, \tag{3.23}$$

$$K_k = \sqrt{\lambda_k} \sum_i m_{ik} A_i. \tag{3.24}$$

This is the operator-sum representation of a quantum operation. Thus, the effective dynamics of a partition of a closed system, which is described by the usual postulates of quantum mechanics, is a quantum operation. Most impressively, the converse is true: any quantum operation in a Hilbert space can be written as unitary dinamics in an extended Hilbert space. The construction of the proof is simple and is done in Ref. [38]. Both proofs together show that Eq. (3.18) is a representation of a quantum operation as valid as Eq. (3.2), and it is called the Stinespring dilation. The extension $\mathbb{H}_B$ of the original system Hilbert space $\mathbb{H}_A$ is called the environment: it is what opens the system out of the closed unitary dynamics. Modeling an environment is usually very hard, however some special cases are treatable and will be done later on.

3.3 Axiomatic definition of a quantum channel

It remains to be proved whether the most general evolution for a quantum state is a quantum operation. It was proved that a quantum state can undergo an evolution more general as an unitary mapping as long as it is part of a bigger structure. Is there yet another generalization? The answer is negative, as we prove in this section. Independently of the nature of a map Φ that is applied on a system ρ, one can argue that it must respect the following axioms:

A1. Normalization: $\operatorname{tr}\Phi[\rho] = \operatorname{tr}\rho = 1$

A2. Linearity: $\Phi[\alpha\rho + \beta\sigma] = \alpha\Phi[\rho] + \beta\Phi[\sigma]$;

A3. Complete positivity: $(\Phi \otimes \mathbb{1})[\rho \otimes \sigma] \geq 0$

These requirements guarantee that Φ transforms a quantum state into a quantum state and that quantum mechanics is a linear theory. Axiom A3 is a lot more subtle than A1 and A2. It states that not only a map on a positive operator ρ should keep it positive, but it also should not break positivity of positive extensions of ρ. This is necessery when the map acts on a subspace of the total Hilbert space, which is arguably always the case for any real quantum state, as experimentalists will never have control over all degrees of freedom of the universe.

A map that fulfills all three axioms is linear and completely positive and trace-preserving (CPTP). In this section we prove that all linear CPTP maps are quantum operations, following the set of notes [47]. Consider that the map acts on Hilbert space $\mathbb{H}_A$, and then construct an exact copy $\mathbb{H}_B$ of this space. Now define the unnormalized state

$$|\Omega\rangle = \sum_i |i\rangle_B \, |i\rangle_A \,, \tag{3.25}$$

where we have ommited the kroneker product for simplicity. Notice that space $\mathbb{H}_B$ was set to the left. With it, we define the Choi matrix of the CPTP map Φ:

$$\Lambda_\Phi = (\mathbb{1} \otimes \Phi)(|\Omega\rangle\langle\Omega|). \tag{3.26}$$

The Choi matrix is a representation of Φ, since it completely characterizes the map [43]:

$$\Phi[\rho] = \mathrm{tr}_B\{(\rho^T \otimes \mathbb{1})\Lambda_\Phi\}, \tag{3.27}$$

where ρ^T is the transpose of ρ. As Φ is CPTP and $|\Omega\rangle\langle\Omega|$ is positive, then Λ_Φ is positive by definition and can be diagonalized:

$$\Lambda_\Phi = \sum_k \lambda_k |\lambda_k\rangle\langle\lambda_k| = \sum_k |m_k\rangle\langle m_k|, \tag{3.28}$$

where we defined $|m_k\rangle = \sqrt{\lambda_k}|\lambda_k\rangle$ for simplicity, making use of the fact that λ_k is positive. Inserting Eq. (3.28) in Eq. (3.27),

$$\Phi[\rho] = \mathrm{tr}_B\{(\rho^T \otimes \mathbb{1})|m_k\rangle\langle m_k|\} = \sum_\alpha \langle\alpha|_B (\rho^T \otimes \mathbb{1})|m_k\rangle\langle m_k||\alpha\rangle_B \tag{3.29}$$

$$= \sum_k \sum_{\alpha,\beta} \langle\alpha|_B (\rho^T \otimes \mathbb{1})|\beta\rangle_B \langle\beta|_B |m_k\rangle\langle m_k||\alpha\rangle_B \tag{3.30}$$

$$= \sum_k \sum_{\alpha,\beta} \rho_{\beta\alpha} \langle\beta|_B |m_k\rangle\langle m_k||\alpha\rangle_B \tag{3.31}$$

Expanding $|m_k\rangle$ in its subspaces, we have

$$|m_k\rangle = \sum_{i,j} (M_k)_{ji} |i\rangle_B |j\rangle_A, \tag{3.32}$$

where M_k is a matrix of the same dimension of the original Hilbert space. Then the term $\langle\beta|_B |m_k\rangle\langle m_k||\alpha\rangle_B$ reads

$$\langle\beta|_B |m_k\rangle = \sum_{ij} (M_k)_{ji} |j\rangle_A \delta_{i\beta} = \sum_j (M_k)_{j\beta} |j\rangle_A, \tag{3.33}$$

$$\langle m_k||\alpha\rangle_B = \sum_{i'j'} (M_k)^*_{j'i'} \langle j'|_A \delta_{i'\alpha} = \sum_{j'} (M_k^\dagger)_{\alpha j'} \langle j'|_A, \tag{3.34}$$

$$\langle\beta|_B |m_k\rangle\langle m_k||\alpha\rangle_B = \sum_{jj'} (M_k)_{j\beta} (M_k^\dagger)_{\alpha j'} |j\rangle_A \langle j'|_A. \tag{3.35}$$

With this Eq. (3.31) is written in terms only of subspace $\mathbb{H}_A$:

$$\Phi[\rho] = \sum_k \sum_{\alpha,\beta} \sum_{j,j'} |j\rangle\, (M_k)_{j\beta} \rho_{\beta\alpha} (M_k^\dagger)_{\alpha j'}\, \langle j'|\,. \tag{3.36}$$

Summing over the completeness relations, we arrive at the desired quantum operation

$$\Phi[\rho] = \sum_k M_k \rho M_k^\dagger. \tag{3.37}$$

This completes the proof. Using only the restriction that Φ is CPTP, we have shown that it can be written in the operator-sum representation and thus is a quantum operation, which in turn shows that a quantum operation is the most general possible transformation a quantum state may go under.

Chapter 4

Quantum coherence

Quantum coherence is a property similar to entanglement in many aspects, nonetheless it does not rely on a partition of the system's Hilbert space. It is associated with the existence of off-diagonal terms in the system density matrix, e.g.

$$\rho = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}. \tag{4.1}$$

Notice that the existence of coherence is basis dependent, as ρ is hermitian and can be diagonalized. Still, as tempting as it may be to define physical quantities in a basis independent fashion, coherence does appeal to reality. For instance, in the previous discussion of Chapter 2, it was stated that a pure state $|\psi\rangle$ retrieves no new information if measured in its diagonal basis. In contrast, if measured in a basis that yields coherence, the measurement results will be non-deterministic in nature. This is an old and well established result in quantum mechanics and is a key concept in truly random number generation [48, 49].

Although such properties are common in the quantum realm, the denizens of the classical world do not experience these features. A natural question then arises: why coherence does not manifest itself in macroscopic systems? As a possible answer to this question, the theory of open quantum systems hints at the necessity of a preferable local basis, and by consequence of a global basis, when many body systems are considered [50]. The mechanism behind that relates to the existence of reservoirs: Hilbert spaces much larger than the system's own Hilbert space, which induce the relaxation of the local system to a target state in a basis imposed by the interaction between the system and reservoir, as will be discussed in Chapter 5.

For now, let us take into account the above discussion and regard coherence as something which is not easy to obtain in practice, and that usual operations in an average laboratory tend to supress it. From this point of view, coherence can be regarded as a valuable resource for some desired task, e.g. random number generation in the previous example.. This approach is formalized in the framework of resource theories [6]. Several resource theories exist, where the resource theory of entanglement [51] is arguably the most famous one.

In this chapter, Section 4.1 will take advantage of the physical appeal of the resource theory of entanglement to develop the basic elements of a general resource theory. Then, in Section 4.2, the resource theory of coherence will be introduced, closely following Ref. [52].

4.1 General resource theories

Resource theories rely on operational constraints imposed by the nature of the experiment done. For instance, suppose the researchers Alice and Bob live in different places, and each of them holds a quantum state that must be isolated by heavy equipment. Alice wants to send Bob her quantum state, but in order for her to do so, she would have to measure it, disturbing it by consequence. Furthermore, the isolating equipment does not allow for the state to be transported from one laboratory to another.

This scenario imposes some constraints on the possible operations for Alice and Bob: since they are isolated from each other, they are only allowed to perform unitary operations on the local systems and to comunicate through classical channels. These operations are called LOCC (Local Operations and Classical Communication). The set of LOCC define all the possible operations they can perform, and thus are dubbed free operations. All states that can be created in the laboratory and achieved from them by free operations are called free states. However, as is well known, a state that is separable cannot be transformed into a non-separable (or entangled) state through local unitaries. Thus, a initially entangled state represents a tool that cannot be created at will and represents a resource. Once the resource is defined, one can pose an important question: How is this resource quantified? For instance, for a given task, such as teleportation, how do different entangled states perform? Is one better than another? Such a question depends on the task at hand. In the above example, an entangled pair shared by Alice and Bob provides them a way to send her quantum state to him without disturbing it through LOCC only [53]. A quantifier that relates to this task will stablish an ordering of the set of entangled states, where its maximum value will correspond to the maximally entangled state. However, not necessarily this ordering will be the same for another quantifier. All these questions permeate the research field not only for the resource theory of entanglement, but of general resource theories [6].

In accordance to what was discussed, there are a couple of properties a good quantifier C must attend in order to quantify resources:

1. C must be 0 for free states;
2. C must be non-increasing under free operations;
3. C must not increase under mixtures of free states.

In summary, what defines a resource theory are the of set free operations, which are the allowed maps of the theory, and the free states, which are those containing no resource.

4.2 Resource theory of coherence

A quantum system that fails to be isolated with perfection suffers decoherence. If the only maps applicable to it are either amplitude dampings or dephasing channels, than coherence in the energy basis becomes a resource. To set this formally as a resource theory, first the free operations and free states must be defined. First, fix a d dimensional basis $\{|j\rangle\}$. Then, for this basis, the set of free states are those of the form

$$\delta = \sum_{j=1}^{d} \delta_j \, |j\rangle \langle j| \, . \tag{4.2}$$

The set of all free states is denoted $\mathbb{I} \subset \mathbb{H}$, where $\mathbb{H}$ is the total Hilbert space. Now, the free operations are those which leave $\mathbb{I}$ invariant. When put in the Kraus representation, the free operations must satisfy

$$K_n \delta K_n^{\dagger} \in \mathbb{I}, \qquad \text{if } \delta \in \mathbb{I} \tag{4.3}$$

for all n. This guarantees that every possible quantum jump will not produce coherence in the free states. With this in hands, one can deal with two different situations. In the first one, the outcome of each jump is not read. For the second one, the outcome is read and post-selection is applied to the state based on the outcome. Although all results derived here apply to both situations, for convenience just the first case is covered here. The incoherent operation described by the action of these Kraus operators on a state ρ will be denoted as

$$\Phi[\rho] := \sum_n K_n \rho K_n^\dagger. \tag{4.4}$$

4.2.1 Maximally coherent state

Here we prove the existence of a state from which one can reach any other state in $\mathbb{H}$ only by means of incoherent operations [52]. Consider the following Kraus operators

$$K_n = \sum_{i=1}^{d} c_i \left|i\right\rangle \left\langle m_{i+n-1}\right|, \tag{4.5}$$

where $\sum_{i=1}^{d} |c_i|^2 = 1$ and $m_k = \mathrm{mod}(k-1, d) + 1$. For concreteness, if $d = 3$ and $n = 2$ we have

$$\begin{aligned} K_2 = \sum_{i=1}^{3} c_i \left|i\right\rangle \left\langle m_{i+2-1}\right| &= c_1 \left|1\right\rangle \left\langle m_2\right| + c_2 \left|2\right\rangle \left\langle m_3\right| + c_3 \left|3\right\rangle \left\langle m_4\right| \\ &= c_1 \left|1\right\rangle \left\langle 2\right| + c_2 \left|2\right\rangle \left\langle 3\right| + c_3 \left|3\right\rangle \left\langle 1\right|. \end{aligned}$$

The set $\{K_n\}$ composes a quantum channel:

$$\sum_{n=1}^{d} K_n^\dagger K_n = \sum_{i,j,n}^{d} c_j^* c_i \left|m_{i+n-1}\right\rangle \left\langle i|j\right\rangle \left\langle m_{j+n-1}\right| = \sum_i^{d} |c_i|^2 \sum_{n=1}^{d} \left|m_{i+n-1}\right\rangle \left\langle m_{i+n-1}\right| = 1. \tag{4.6}$$

Let us now show that this channel is a free operation:

$$K_n \delta K_n^\dagger = \sum_{i,j,k=1}^{d} c_i c_j^* \delta_k \left|i\right\rangle \left\langle m_{i+n-1}\right|k\rangle \langle k\left| m_{j+n-1}\right\rangle \left\langle j\right| = \sum_{i=1}^{d} |c_i|^2 \delta_{m_{i+n-1}} \left|i\right\rangle \left\langle i\right| \in \mathbb{I}. \tag{4.7}$$

Notice that the set formed by the Kraus operators (4.5) forms a family of maps parametrized by the coefficients c_i. One can always define a convex mixture of the members these families, for instance with additional parameters q_l, such that one still has an incoherent operation:

$$K_n^{(l)} = \sqrt{q_l} K_n, \tag{4.8}$$

$$K_n^{(l)} \rho K_n^{(l)\dagger} = q_l K_n \rho K_n^\dagger, \tag{4.9}$$

$$\sum_l q_l = 1. \tag{4.10}$$

With this map at hand, we are now in position to define the maximally coherent state $|\Psi\rangle$:

$$|\Psi\rangle = \frac{1}{\sqrt{d}} \sum_{j=1}^{d} |j\rangle \,. \tag{4.11}$$

If the map (4.5) is applied to (4.11), one gets

$$K_n |\Psi\rangle = \frac{1}{\sqrt{d}} \sum_{j=1}^{d} c_j \sum_{i=1}^{d} |j\rangle \langle m_{j+n-1}| i\rangle = \frac{1}{\sqrt{d}} \sum_{j=1}^{d} c_j |j\rangle := \frac{1}{\sqrt{d}} |\phi\rangle \,, \tag{4.12}$$

$$\rho_n = \frac{1}{p_n} K_n |\Psi\rangle \langle\Psi| K_n^\dagger = d\frac{1}{d} |\phi\rangle \langle\phi| = |\phi\rangle \langle\phi| \,. \tag{4.13}$$

Since the result is the same for every n, then $p_n = {}^1\!/_d$. The c_j are arbitrary up to normalization, henceforth $|\phi\rangle$ is a general pure state. By means of definition (4.8), one can write any mixture of different pure states $|\phi^{(l)}\rangle$:

$$K_n^{(l)} |\Psi\rangle \langle\Psi| K_n^{(l)\dagger} = \frac{1}{d} q_l |\phi^{(l)}\rangle \langle\phi^{(l)}| \tag{4.14}$$

$$\rho = \sum_l q_l |\phi^{(l)}\rangle \langle\phi^{(l)}| \,. \tag{4.15}$$

With this, one can achieve any arbitrary quantum state ρ [38]. This completes the proof, as was shown that any mixed state can be prepared by means of $|\Psi\rangle$ and incoherent operations.

4.2.2 Coherence measures

After the maximally coherent state and the incoherent states are defined, one wonders what are the states in between. This motivates the definition of coherence measures C that stablish an ordering of the states. Inspired by the properties a good quantifier should have, we define the following properties:

(C1) $C(\rho) = 0 \quad \text{iff} \quad \rho \in \mathbb{I}$,

(C2) $C(\rho) \geq C(\Phi[\rho])$.

Property C1 ensures that the measure is 0 if only if the the state is incoherent. Some resource theories allow for a weaker condition, where the measure is 0 for every free state but the converse need not be true, such as negativity for entangled states [6]. This is usually done when a measure that both respect C1 and is efficiently computable is not known. This will not be the case for coherence.

Property C2 establishes an ordering of the states in the sense of the given measure. After an incoherent operation, coherence can only decrease or stay the same. This corroborates with a notion of a resource: one either consumes it or converts it to an equivalent quantity.

As a stating point to define measures from coherence, one can relate existing metrics to the task at hand [54,55]:

$$C_D(\rho) = \min_{\delta \in \mathbb{I}} D(\rho, \delta). \tag{4.16}$$

The strategy is to use an existing distance D used on quantum states and minimize it with respect to the incoherent set. Then, one figures what properties D must have in order for C to fulfill conditions C1 and C2.

For C1 to be fulfilled, the only requirement is that $D(\rho, \delta) = 0$ iff $\rho = \delta$. This is satisfied by several measures, in particular for the relative entropy (2.7) and all metrics.

If the distance D is contractive under CPTP maps, then C2 is fulfilled:

$$C_D(\rho) = D(\rho, \delta^*) \geq D(\Phi[\rho], \Phi[\delta^*]) \geq \min_{\delta \in \mathbb{I}} D(\Phi[\rho], \delta) = C_D(\Phi[\rho]), \tag{4.17}$$

where in the first equality δ^* is the element of $\mathbb{I}$ that minimizes Eq. (4.16), the second equality defines contractiveness, and the third equality is a second minimization over the space $\mathbb{I}$, which is possible since $\Phi[\delta^*] \subset \mathbb{I}$ by definition.

Eq. (2.7) is contractive under CPTP maps [56], and thus a measure derived from it respects both C1 and C2. Incidently, the relative entropy provides an analytical structure for Eq. (4.16) that requires no minimization. First, define the diagonal of a state ρ as ρ_{diag}:

$$\rho = \sum_{i,j=1}^{d} \rho_{ij} \left| i \right\rangle \left\langle j \right|, \tag{4.18}$$

$$\rho_{\text{diag}} = \sum_{i=1}^{d} \rho_{ii} \left| i \right\rangle \left\langle i \right|. \tag{4.19}$$

Then, from the definition of relative entropy and of an incoherent state δ,

$$\begin{aligned} S(\rho \| \delta) &= -S(\rho) - \text{tr}\{\rho \log \delta\} = -S(\rho) - \sum_i \langle i | \rho \log \delta | i \rangle & (4.20) \\ &= -S(\rho) - \sum_i \rho_{ii} \log \delta_i = -S(\rho) - \text{tr}\{\rho_{\text{diag}} \log \delta\} & (4.21) \\ &= -S(\rho) + S(\rho_{\text{diag}}) + S(\rho_{\text{diag}} \| \delta). & (4.22) \end{aligned}$$

Now, using the relative entropy as D, and noting that $\rho_{\text{diag}} \subset \mathbb{I}$:

$$C_{\text{rel}} = \min_{\delta \in \mathbb{I}} S(\rho \| \delta) = \min_{\delta \in \mathbb{I}} (-S(\rho) + S(\rho_{\text{diag}}) + S(\rho_{\text{diag}} \| \delta)) = S(\rho_{\text{diag}}) - S(\rho), \tag{4.23}$$

where in the last equality Eq. (2.8) was used. The monotone C_{rel} derived is named entropy of coherence, and will be used extensively in Chapter 6. Its importance lies mainly on its entropic nature, which allows for a link between the resource theory of coherence and thermodynamics, and on its form, which is analytical and easily computable.

As a sidenote, property C2 is cast differently when post-selection is allowed, for the map (4.4) changes. Proving C2 is harder in this case, as no general result such as the contractiveness exists. C_{rel} does respect the more restrictive condition [52], but as no post-selection will be used further on, we have chosen to omit this discussion.

Chapter 5

Master equation formalism

In Chapter 3 the formalism of quantum operations was developed, where it was shown that the evolution of a quantum system may be generalized to any CPTP map as long as it is part of a larger system. Until then, the operator-sum representation had a major focus as its form is quite simple and easy to manipulate. However, the channel becomes a black box in this representation, as only its input and output are visible. The Stinespring dilation is a valid alternative to look at the dynamics, but even mesoscopic environments already render the extension's Hilbert space unwieldly large: it grows exponentially with the number of particles.

The focus of this chapter is to develop tools for the treatment of large environments, reservoirs such as thermal baths. It is shown that, under certain conditions, the degrees of freedom of the reservoir are compressed into an additional structure in the reduced von Neumann equation for the system. This structure is called the master equation, or Gorini-Kossakowski-Sudarshan-Lindblad equation (GKSL equation), and will be introduced in the first section [56, 57]. Then, in the next section, we show how to achieve this equation from first principles with a so called microscopic derivation [46].

5.1 Master equations

The master equation is a linear differential equation for a quantum system ρ:

$$\dot{\rho} = \mathcal{L}\rho := -i[H, \rho] + \mathcal{D}[\rho], \tag{5.1}$$

$$\mathcal{D}[\rho] = \sum_k \gamma_k D[L_k], \tag{5.2}$$

$$D[L_k] = L_k \rho L_k^\dagger - \frac{1}{2}\{L_k^\dagger L_k, \rho\}. \tag{5.3}$$

The superoperator $\mathcal{L}$ is often called the Liouvillian. Superoperators have the same properties as operators, but they act on operators instead of states. For that matter, although they have matrix representation on the vector space formed by operators, in the vector space formed by states they need matrices acting on both sides of operators to be represented.

Eq. (5.1) is the same as the von Neumann equation, except for the operators (5.3). Their action on the system induce dissipative dinamics on ρ, and thus are called dissipators. The operators L_k composing them are called jump operators. The coefficients γ_k are the damping rates. The GKSL equation destroys some subspaces of the system's original Hilbert space, and its decay rate is associated with a γ_k, justifying their name [46]. The dissipative term $\mathcal{D}[\rho]$ must be traceless in order for Eq. (5.1) to remain trace preserving. For the individual $D[L_k]$, one can always find L_k such that they are all traceless [46].

It is important to stress that this kind of evolution is not general. If we have a structured Hilbert space $\mathbb{H} = \bigotimes_n \mathbb{H}_n$, the global evolution is described by a the von Neumann equation. However, when we treat the local dynamics in a given subspace $\mathbb{H}_n$, their evolution cannot be necessarily cast as a differential (or master) equation. The most general evolution, as we saw before, is a quantum channel. The connection between channels and master equations, and the requirements for such a channel to be cast in a differential representation are throughly discussed in Ref. [58]. The main requirement is that the channel must be invertible.

As an example of master equation, we write the action of a thermal bath on a qubit, a channel refered to as amplitude damping:

$$\dot{\rho} = -i\omega[\sigma^\dagger\sigma, \rho] + \gamma D[\sigma]. \tag{5.4}$$

This is an amplitude damping to a thermal bath of temperature 0. We expect the solution to be unique, a steady state relaxation towards a thermal state of same temperature as the reservoir's. The damping rate γ gives the timescale for the relaxation to the said steady state. The uniqueness of solutions is not a general property of all master equations, however is true for the majority of cases. The existence of more than one steady state is related to strong symmetries in the Lindbladian [59, 60].

To solve a master equation, the simplest way to proceed is to just write the set of linear differential equations for the components of the density matrix and solve them, as long as the dimension is finite. The linear system in Eq. (5.4) case reads

$$\dot{\rho}_{11} = -\gamma\rho_{11}, \tag{5.5}$$

$$\dot{\rho}_{12} = (-i\omega - \gamma/2)\rho_{12}. \tag{5.6}$$

Here we just need equations for ρ_{11} and ρ_{12}, for $\rho_{22} = 1 - \rho_{11}$ and $\rho_{21} = \rho_{12}^*$. The solution for these equations is

$$\rho_{11} = e^{-\gamma t}, \tag{5.7}$$

$$\rho_{12} = e^{-(i\omega+\gamma/2)t}. \tag{5.8}$$

As expected, the population of the excited state decreases exponentially to 0. The coherences do the same, although oscillating as an effect of the free Hamiltonian. The steady state ρ_{ss} is then the ground state.

Not always the system of differential equations is easy to solve. The equations are generally coupled, and in higher dimensions the dynamics may become impossible to compute efficiently. In these cases, one can still compute the steady state. Notice that the existence of a staedy state implies that $\lim_{t\to\infty}\dot{\rho}(t) = 0$. Then the equations become algebraic and effeciently solved numerically.

Let us refer back to Eq. (5.4). In it, there is a single dissipator associated with the jump operator σ. Now consider the case in which $D[\sigma^\dagger]$ is also present. The new equation reads

$$\dot{\rho} = -i\omega[\sigma^\dagger\sigma, \rho] + \gamma(1-f)D[\sigma] + \gamma f D[\sigma^\dagger]. \tag{5.9}$$

The constant f just enables different weights for both dissipators, while still preserving the trace of ρ. The differential equations for Eq. (5.9) are

$$\dot{\rho}_{11} = -\gamma(1-f)\rho_{11} + \gamma f(1-\rho_{11}), \tag{5.10}$$

$$\dot{\rho}_{12} = (-i\omega - \gamma/2)\rho_{12}. \tag{5.11}$$

The equation for coherences is the same, in contrast with the equation for populations. Ignoring the dynamics, the stady state for ρ_{11} is now f. It is still thermal, but with nonzero effective temperature. Eq. (5.9) is the amplitude damping channel for finite temperature. Although this is trivial in the sense that every diagonal qubit state is a thermal state, it generalizes properly for higher dimensions.

From these examples one can draw some general conclusions on how the choice of jump operators affect the dynamics of the system: they represent the transitions induced by the environment on the system. When the environment induces solely a σ transition, the system eventually decays to the ground state. However, if the transition $\sigma^\dagger$ is also enabled, the system will relax to a thermal state produced by the balance between the dissipators, characterized by f. This assertion will be made more precise in Sec. **??**. But, from a qualitative perspective, the relevant message is that jump operators represent the transitions induced by the bath on the system. This provides useful guidelines when constructing phenomenological dissipators. For example, if one would be interested in the dynamics of a harmonic oscillator in contact with a thermal bath, a first phenomenological approach would be to just write a master equation with creation and anihillation operators $a^\dagger$ and a as the jump operators for the dissipators.

5.2 Microscopic derivation of a master equation

Previously the master equation for an amplitude damping channel on a qubit was shown, but it was not ellucidated how one would derive it from first principles. The problem to be solved is the dynamics of a system ρ_S that lives on a Hilbert space $\mathbb{H}_S$, which in turn is part of a much larger Hilbert space $\mathbb{H} = \mathbb{H}_S \otimes \mathbb{H}_E$, where ρ lives on and evolves unitarily. The state of the environment ρ_E is the projection of ρ into $\mathbb{H}_E$. Moreover, at $t = 0$ the system and the reservoir are uncorrelated, and hence $\rho(0) = \rho_S(0)\rho_E$. The chosen method provides a general procedure to derive a microscopic master equation for ρ_S, with clear physical motivation. It is called Nakajima-Zwanzig method [61, 62], which relies on the definition of the projector $\mathcal{P}$ defined below:

$$\mathcal{P}\rho(t) = \mathrm{Tr_E}\{\rho(\mathrm{t})\}\rho_\mathrm{E}(0) = \rho_\mathrm{S}(\mathrm{t}) \otimes \rho_\mathrm{E}(0). \tag{5.12}$$

The idea is to write the evolution of $\mathcal{P}$, changing the problem of evolving a state to that of evolving a subspace. It is easily seen that $\mathcal{P}$ is indeed a projector, since

$$\mathcal{P}^2\rho(t) = \mathcal{P}(\rho_S(t) \otimes \rho_E(0)) = \rho_S(t) \otimes \rho_E(0) = \mathcal{P}\rho(t) \tag{5.13}$$

and thus $\mathcal{P}^2 = \mathcal{P}$.

Before proceeding, some remarks on the evolution of ρ. The total Hamiltonian of the system is $H = H_S + H_E + V$, where H_S and H_E are the respective free Hamiltonians for the system and environment, and V is the interaction between them. We work on the interaction picture with respect to the free Hamiltonians:

$$\frac{d}{dt}\tilde{\rho} = -i[\tilde{V}, \tilde{\rho}], \tag{5.14}$$

where $\tilde{\rho}(t) = e^{i(H_S+H_E)t}\rho(t)e^{-i(H_S+H_E)t}$ and $\tilde{V}(t) = e^{i(H_S+H_E)t}Ve^{-i(H_S+H_E)t}$. The tildes are dropped in the following calculations to make the equations clearer. In the end, one can go back to the Schrdinger picture. The interaction here is chosen to satisfy

$$\mathrm{Tr_E}\{\mathrm{V}\rho_\mathrm{E}\} = 0, \tag{5.15}$$

where this implies that the interaction between system and environment does not retain energy, and thus changes in energy on the environment are completely transfered to the system. It is not a limitation of the method, in fact this is chosen so that thermodynamics can be drawn from this later on. The reason for the necessity of the condition (5.15) to thermodynamics is that energy retained in the interaction cannot be labelled neither as system energy nor as reservoir energy, turning it difficult to define work and heat [21].

All the necessary tools are assembled to treat the problem. Consider first the evolution of the two orthogonal subspaces of $\mathbb{H}$ defined by $\mathcal{P}$ and $\mathcal{Q} = 1 - \mathcal{P}$:

$$\frac{d}{dt}\mathcal{P}\rho(t) = \mathcal{P}\mathcal{V}_t\rho(t), \tag{5.16}$$
$$\frac{d}{dt}\mathcal{Q}\rho(t) = \mathcal{Q}\mathcal{V}_t\rho(t), \tag{5.17}$$

where $\mathcal{V}_t = -i[V(t), \cdot\ ]$ is the superoperator associated with unitary evolution. In order to write the evolution of the subspaces as coupled differential equations, a unity $1 = \mathcal{P}+\mathcal{Q}$ is put between $\mathcal{V}_t$ and $\rho(t)$:

$$\frac{d}{dt}\mathcal{P}\rho(t) = \mathcal{P}\mathcal{V}_t\mathcal{P}\rho(t) + \mathcal{P}\mathcal{V}_t\mathcal{Q}\rho(t), \tag{5.18}$$

$$\frac{d}{dt}\mathcal{Q}\rho(t) = \mathcal{Q}\mathcal{V}_t\mathcal{P}\rho(t) + \mathcal{Q}\mathcal{V}_t\mathcal{Q}\rho(t). \tag{5.19}$$

These coupled equations can be mapped to

$$\dot{x}(t) = A(t)(x(t) + y(t)), \tag{5.20}$$

$$\dot{y}(t) = B(t)(x(t) + y(t)), \tag{5.21}$$

where A and B are superoperators and x and y are operators. The formal solution to $y(t)$ is

$$y(t) = G(t, t_0)y(0) + \int_0^t dt' G(t, t')B(t')x(t'), \tag{5.22}$$

$$G(t, t_0) = \mathcal{T}\exp\left\{\int_{t_0}^t dsB(s)\right\}, \tag{5.23}$$

where $G(t, t_0)$ is the Green's function for Eq. (5.21) and $\mathcal{T}$ is the time-ordering operator. Since $y(0) = \mathcal{Q}\rho(0)$ and $\rho(0) = \rho_S(0)\rho_E$ lives by definition on the projection $\mathcal{P}$, $y(0) = 0$. Substituting these in Eq. (5.20),

$$\dot{x}(t) = A(t)x(t) + \int_0^t dt' A(t)G(t, t')B(t')x(t'). \tag{5.24}$$

The first term can be written as

$$A(t)x(t) = \mathcal{P}\mathcal{V}_t\mathcal{P}\rho(t) = \mathcal{P}\mathcal{V}_t\rho_S(t)\rho_E. \tag{5.25}$$

Expanding $\mathcal{V}_t$ and using the first equality of Eq. (5.12),

$$\mathcal{P}\mathcal{V}_t\rho_S(t)\rho_E = -i\mathcal{P}[V(t), \rho_S(t)\rho_E] = \mathrm{Tr_E\{-i[V(t), \rho_S(t)\rho_E]\}\rho_E}. \tag{5.26}$$

Using Eq. (5.15),

$$\mathrm{Tr_E\{[V(t), \rho_S(t)\rho_E]\} = Tr_E\{V(t)\rho_E]\}\rho_S(t) + \rho_S(t)Tr_E\{V(t)\rho_E]\} = 0}. \tag{5.27}$$

Thus, $A(t)x(t) = \mathcal{P}\mathcal{V}_t\mathcal{P} = 0$ and Eq. (5.24) reads

$$\dot{x}(t) = \int_0^t dt' A(t)G(t,t')B(t')x(t') = \int_0^t dt' \mathcal{P}\mathcal{V}_t G(t,t')\mathcal{Q}\mathcal{V}_{t'}\mathcal{P}\rho(t') \tag{5.28}$$

$$= \int_0^t dt' \mathcal{P}\mathcal{V}_t G(t,t')(1-\mathcal{P})\mathcal{V}_{t'}\mathcal{P}\rho(t') = \int_0^t dt' \mathcal{P}\mathcal{V}_t G(t,t')\mathcal{V}_{t'}\mathcal{P}\rho(t'). \tag{5.29}$$

Hence, in the end the time evolution of the $\mathcal{P}$ projection of ρ is obtained:

$$\frac{d}{dt}\mathcal{P}\rho(t) = \int_0^t dt' \mathcal{P}\mathcal{V}_t G(t,t')\mathcal{V}_{t'}\mathcal{P}\rho(t'). \tag{5.30}$$

This is named the Nakajima-Zwanzig equation, and is exact for the local state of the system. Nevertheless the true final state of the reservoir is not known, for it is contained inside the subspace represented by the projector $\mathcal{Q}$ that was integrated out in Eq. (5.23). The projector $\mathcal{P}$ outputs a state for the reservoir that is both uncorrelated with the system and unchanged by the dynamics. This state becomes a good approximation when the reservoir is large enough, or if the coupling is weak enough [46]. However, even when the assumption of small correlation between system and environment is true, it is still quintessential for the dynamics. The main reason is that there is a general consensus that a system only thermalizes because of its correlations with its environment [63]. The most famous type of correlation in this context is entanglement, however there are examples where system relaxation occurs when no entanglement between S and E is present [64].

Weak coupling has yet another consequence on the Nakajima-Zwanzig equation. Suppose this assumption is materialized by scaling V, and by consequence $\mathcal{V}_t$, by a infinitesimal factor ϵ. Then Eq. (5.30) becomes

$$\frac{d}{dt}\mathcal{P}\rho(t) = \epsilon^2 \int_0^t dt' \mathcal{P}\mathcal{V}_t G(t,t')\mathcal{V}_{t'}\mathcal{P}\rho(t'). \tag{5.31}$$

Now, as ϵ is infinitesimal, we may expand $G(t,t')$ around $\epsilon = 0$:

$$G(t,t_0) = \mathcal{T}\exp\left\{\int_{t_0}^t ds B(s)\right\} = \mathcal{T}\exp\epsilon\left\{\int_{t_0}^t ds \mathcal{Q}\mathcal{V}_s\right\} = \mathbb{1} + \mathcal{O}(\epsilon), \tag{5.32}$$

where $\mathcal{O}(\epsilon)$ denotes any terms of order ϵ. If Eq. (5.31) is to be mainteined of order ϵ^2, then

$$\frac{d}{dt}\mathcal{P}\rho(t) = \epsilon^2 \int_0^t dt' \mathcal{P}\mathcal{V}_t\mathcal{V}_{t'}\mathcal{P}\rho(t'). \tag{5.33}$$

This is often called the Born approximation, a frequent assumption of the weak coupling limit [46]. It is very useful, as the Green's function is model dependent and highly non-trivial to calculate. To set it as unity pushes the general result further while simplifying it. Eq. (5.33) is known as the Redfield equation [65].

Although the Redfield equation is indeed simpler than Eq. (5.30), it is still hindering because of its time non-local structure: the rate of change of $\mathcal{P}\rho$ at time t depends on the entire history of the state's dynamics, as can be seen from $\rho(t')$ inside the time integral. This evokes the concept of memory, i.e. the dynamics rely on the memory the system has about its previous states. Such dynamics is named non-Markovian, where Markovianity is thus defined as lack of memory. As a revervoir is supposed to be much larger than the system, one would expect that it should hold no memory of it. This motivates the Markovian approximation, where Eq. (5.33) is forced to be local in time by exchanging $\rho(t')$ by $\rho(t)$:

$$\frac{d}{dt}\mathcal{P}\rho(t) = \epsilon^2 \int_0^t dt' \mathcal{P}\mathcal{V}_t\mathcal{V}_{t'}\mathcal{P}\rho(t). \tag{5.34}$$

This is still time non-local, for the integral still depends on $t = 0$. To supress this dependance, first make the transformation of variables $t' = t - s$

$$\frac{d}{dt}\mathcal{P}\rho(t) = \epsilon^2 \int_0^t ds \mathcal{P}\mathcal{V}_t\mathcal{V}_{t-s}\mathcal{P}\rho(t), \tag{5.35}$$

and then take the limit where the integral goes to infinity:

$$\frac{d}{dt}\mathcal{P}\rho(t) = \epsilon^2 \int_0^\infty ds \mathcal{P}\mathcal{V}_t\mathcal{V}_{t-s}\mathcal{P}\rho(t). \tag{5.36}$$

Now, the integral has no dependence on the initial state. The manipulations on the Born-Markov Nakajima-Zwanzig equation are over, it remains only to incorporate ϵ back into $V(t)$ and expand the superoperators in order to turn the equation operational:

$$\frac{d}{dt}\mathrm{Tr_E}\{\rho(\mathrm{t})\}\rho_\mathrm{E} = \int_0^\infty \mathrm{ds}\ \mathrm{Tr_E}\{(-\mathrm{i})[\mathrm{V(t)}, (-\mathrm{i})[\mathrm{V(t-s)}, \mathrm{Tr_E}\{\rho(\mathrm{t})\}\rho_\mathrm{E}]]\}\rho_\mathrm{E}, \tag{5.37}$$

$$\Rightarrow \dot{\rho}_S(t) = -\int_0^\infty ds\ \mathrm{Tr_E}[\mathrm{V(t)}, [\mathrm{V(t-s)}, \rho_\mathrm{S}(\mathrm{t})\rho_\mathrm{E}]]. \tag{5.38}$$

This is as far as a model independent analysis can reach. To proceed further, one must assume a form for both V and ρ_E. As an interesting sidenote, it can be shown that Eqs. (5.33) and (5.34) are the same up to order $O(\epsilon^2)$ [46]. Although not exactly the same, both present a deviation of the same order of magnitude to the exact solution for any given model.

An example in which this formulation proves useful is a qubit trading quanta with a bath of non-interacting harmonic oscilators:

$$H = H_0 + V, \tag{5.39}$$

$$H_0 = \omega\sigma^\dagger\sigma + \sum_k \Omega_k a_k^\dagger a_k, \tag{5.40}$$

$$V = \sum_k g_k \sigma a_k^\dagger + g_k^* \sigma^\dagger a_k, \tag{5.41}$$

where $\{\omega, \Omega_k\}$ are the natural frequencies of the qubit and oscillators, $\{\sigma, a_k\}$ the anihillation operators of a quanta in the qubit and of a boson in each individual mode, and g_k the coupling between each qubit - oscillator interaction. This is Hamiltonian is used for many quantum optics and condensed matter settings, such as atom-light interaction [66] and phonons in lattices [67]. When all $\Omega_k = \omega$, the interaction takes energy from the qubit and retrives the same energy to the oscilators, and thus it preserves energy. Indeed, using the algebra of bosons and Pauli matrices, it is straghtforward to show that $[H_0, V] = 0$. Eq. (5.34) to study this model when the initial state of the bath is thermal. The through calculations are out of the scope of this discussion and can found in Ref. [46]:

$$\dot{\rho}_S(t) = -i[\omega' \sigma^\dagger\sigma, \rho_s(t)] + \mathcal{D}[\rho_S], \tag{5.42}$$

$$\mathcal{D}[\rho_S] = \gamma\bar{n}\left[\sigma^\dagger\rho_S\sigma - \frac{1}{2}\{\sigma\sigma^\dagger, \rho\}\right] + \gamma(\bar{n}+1)\left[\sigma\rho_S\sigma^\dagger - \frac{1}{2}\{\sigma^\dagger\sigma, \rho\}\right], \tag{5.43}$$

where $\bar{n}$ is the the thermal occupation number of bosons in the bath and γ is related to the interaction between the qubit and each mode of the bath. It is of the GKSL form, as expected.

Chapter 6

Collisional models

In Chapter 5, we have shown that under some approximations one can model a system opened to a large environment through the GKSL equation. However, two main problems arise: the approximations are often severe, leading to unphysical situations [68]; the master equation formalism loses track of the environment degrees of freedom, mining the possibility of using quantum information methods to understand how information about the system propagates into the environment. To this end, we develop here the formalism of collisional models, or repeated interactions [16, 21, 69]. It offers a bottom-top description of an environment, where one has precise theoretical control of the microscopic aspects that give rise to macroscopic characteristics of the bath. The first section is devoted to a detailed description of what is a collisional model. The following section connects the model with master equations, providing the main ingredients for reservoir engineering in the Markovian regime [21]. Then, in a later section, thermodynamics is discussed inside the collisional model while making use of information-theoretic tools developed in Chapter 2 [21]. The chapter closes with the novelty provided by this dissertation: the role of coherence in these models, along with its connection to Hamiltonian engineering, thermodynamics, and resource interconversion [32].

6.1 The collisional model

The collisional model can be seen as a quantum algorithm acting on the system of interest ρ_S. First, the system couples to an ancilla ρ_{A_n}. Then, they evolve through a unitary U_n for a certain time τ and decouple. Finally, we dischart the ancilla and repeat the process with $\rho_{A_{n+1}}$ and U_{n+1}.

A cartoon of the algorithm is shown in Fig. 6.1. The algorithm is described by the map

$$\Phi = \Lambda_N \cdots \Lambda_1, \tag{6.1}$$

$$\Lambda_n[\rho_S] = \mathrm{Tr}_{\mathrm{A_n}}\{\mathrm{U_n}(\tau)(\rho_\mathrm{S} \otimes \rho_{\mathrm{A_n}})\mathrm{U_n^\dagger}(\tau)\}. \tag{6.2}$$

For simplicity, unless otherwise especified, we use identical ancillae and interactions from now on:

$$\Phi = \Lambda^N, \tag{6.3}$$

$$\Lambda[\rho_S] = \mathrm{Tr_A}\{\mathrm{U}(\tau)(\rho_\mathrm{S} \otimes \rho_\mathrm{A})\mathrm{U}^\dagger(\tau)\}. \tag{6.4}$$

However, most of the results derived in the following sections still hold for the general map Eq. (6.1). As we will frequently make use this equation, we set here $\rho'_S = \Lambda[\rho_S]$ to clean up the notation. From now on, every time a quantity is primed, it will be the one related to the referenced system after the interaction. Moreover, Δ denotes the variation from the unprimed to the primed quantity.

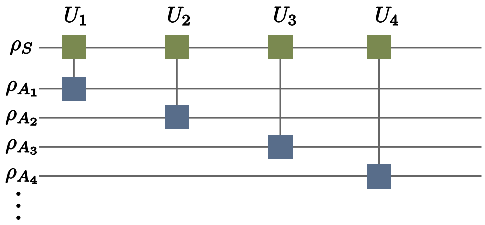

Figure 6.1: A quantum circuit view of the collisional model. After the interaction, the corresponding ancilla is ignored and thus the system is governed by an effective non-unitary map.

The full dynamics is unitary, where the full state is $\rho = \rho_S \bigotimes_{n=1}^N \rho_A$. Thus, the collisional model is a Stinespring dilation process for ρ_S. Since we admit only two body interactions (assuming the system and ancillae have no structure), we have several sequential interaction Hamiltonians V, living in different Hilbert spaces. However, although it is an abuse of notation, we choose not to address this detail and consider them to be the same, since it will not affect the results. The same will be done with the label A for the identical ancillae.

The free parameters are the ancillae chosen and the type of interaction the system holds with them. Notice that Eq. (6.3) is Markovian by construction, given its divisible structure in the equal maps. It can be generalized to non-Markovian dynamics by making the subsequent maps correlated [70], the initial state of the ancillas correlated [71], by utilizing the same ancilla more than one time [72] and ancilla-ancilla interactions [73]. However, this is out of the scope of this dissertation.

6.2 Reservoir engineering

Master equations are differential, Eq. (6.3) is in contrast discrete. In order to bridge them, we perform a series expansion on the map, as we later on intend to take the continuum limit $\tau \to 0$. The interaction, up to order τ^2, reads

$$U(\tau) = \exp\{-iH\tau\} = \mathbb{I} - i\tau H - \frac{\tau^2}{2}H^2,$$

where $H = H_0 + V$ is the total Hamiltonian and H_0 is the free Hamiltonian. We can decompose H_0 further into the free Hamiltonian H_S of the system S and H_A of the ancillae A. Manipulating the expansion above, we get

$$\rho'_S = U(\tau)\rho U^\dagger(\tau) = \rho - i\tau[H,\rho] - \frac{\tau^2}{2}[H,[H,\rho]]. \tag{6.5}$$

Next we take the partial trace with respect to A. The first term returns ρ_S by definition. For the second term,

$$\begin{aligned}\mathrm{Tr_A[H,\rho]} &= [H_S,\rho_S]\mathrm{Tr_A}\rho_\mathrm{A} + \rho_\mathrm{S}\mathrm{Tr_A[H_A,}\rho_\mathrm{A}] + \mathrm{Tr_A[V,}\rho_\mathrm{S}\otimes\rho_\mathrm{A}]\\ &= [H_S,\rho_S] + [G,\rho_S] = [H_S + G,\rho_S],\end{aligned}$$

where we used normalization, that the trace of a commutator with the density matrix is always 0, and defined

$$G := \mathrm{Tr_A\{V}\rho_\mathrm{A}\}. \tag{6.6}$$

For the last term, we can use the same procedure to show that

$$\begin{aligned}\mathrm{Tr_A[H,[H,}\rho]] &= [H_S,[H_S,\rho_S]] + [V,[V,\rho_S]]\\ &= -2H_S\rho_S H_S + \{H_S^2,\rho_S\} - 2V\rho_S V + \{V^2,\rho_S\}.\\ &= \mathcal{D}_H[\rho_S] + \mathcal{D}_V[\rho_S],\end{aligned} \tag{6.7}$$

where

$$\mathcal{D}_H[\rho_S] := -\frac{1}{2}\mathrm{Tr_A}[\mathrm{H_S}, [\mathrm{H_S}, \rho]], \tag{6.8}$$
$$\mathcal{D}_V[\rho_S] := -\frac{1}{2}\mathrm{Tr_A}[\mathrm{V}, [\mathrm{V}, \rho]]. \tag{6.9}$$

These two terms will be related to dissipators later on. We do antecipate that $\mathcal{D}_H[\rho_S]$ produces dephasing in the local energy basis of the system and that $\mathcal{D}_V[\rho_S]$ is a dissipator where the jump operators are related to the interaction V. Eq. (6.5) will thus read

$$\rho'_S = \rho_S - i\tau[H_S + G, \rho_S] + \tau^2\mathcal{D}_H[\rho_S] + \tau^2\mathcal{D}_V[\rho_S]. \tag{6.10}$$

We traverse to the continuum limit by defining

$$\dot{\rho}_S := \lim_{\tau\to 0}\frac{\rho'_S - \rho_S}{\tau}. \tag{6.11}$$

Manipulating Eq. (6.10), we get

$$\frac{\rho'_S - \rho_S}{\tau} = -i[H_S + G, \rho_S] + \tau\mathcal{D}_H[\rho_S] + \tau\mathcal{D}_V[\rho_S]. \tag{6.12}$$

If we take the limit $\tau \to 0$, we lose the desired dissipative effect of Eqs. (6.8) and (6.9). We can solve this problem by inspiring on classical stochastic mechanics, in particular on the Langevin equation description of Brownian motion [74]:

$$m\ddot{\mathbf{x}} = -\lambda\dot{\mathbf{x}} + \eta, \tag{6.13}$$

where η is a random force done by impinging particles constituting a viscous medium of damping λ on a body of mass m and and position $\mathbf{x}$. This random force's distribution is proportional to a delta function and is responsible for the diffusive effect, which would otherwise be damped by the media. The ideia is that, in order for kicks of infinitelly small duration to have a finite effect, they must be equally infinitely strong.

We can use the same idea by rescaling the interaction Hamiltonian as $V \to V/\sqrt{\tau}$. Other scalings are either trivial or diverge [18]. This leads to

$$\frac{\rho'_S - \rho_S}{\tau} = -i[H_S + \frac{G}{\sqrt{\tau}}, \rho_S] + \tau\mathcal{D}_H[\rho_S] + \mathcal{D}_V[\rho_S], \tag{6.14}$$

since $G \propto V$ and $\mathcal{D}_V[\rho_S] \propto V^2$. The scaling solves the problem for the dissipative effect, but opens a divergence in the effective Hamiltonian G. This is the crucial point to develop the main objective of the whole text, which will be treated in the last section. However, we can still work around this issue by considering that $G = 0$, in other words, that the possible diagonal elements of V were incorporated in H_0 and that ρ_A is diagonal in the energy basis. This can be seen from Eq. (6.6): the product of a diagonal matrix with hollow matrix[1] is a hollow matrix, and thus the trace is 0. Furthermore, the dephasing effect remains of order τ and will not contribute to the dynamics in the continuum limit. For that reason, we drop the subscript of the remaining dissipator to clean up the notation and write

$$\dot{\rho}_S = -i[H_S, \rho_S] + \mathcal{D}[\rho_S]. \tag{6.15}$$

We arrived at a master equation, where the dissipative term has the interaction V and the diagonal state ρ_A as a free parameters.

For future reference, we can use the fact the interaction is symmetrical to write the map for A:

$$\rho_A' = \rho_A - i\tau[H_A + G_A/\sqrt{\tau}, \rho_A] + \tau\mathcal{D}_A[\rho_A], \tag{6.16}$$

where G_A and $\mathcal{D}_A$ are defined as G and $\mathcal{D}$, but replacing A with S and vice versa. Notice that since we want our system to be arbitrary, G_A is not 0.

6.2.1 Energy preserving interactions and its parametrization

To visualize how one can perform bath engineering, we consider the special case of energy preserving interactions. This allows us to explicitly parametrize V and thus write the dissipator in a familiar form. When the interaction is energy preserving, we can always write it as

$$V = \sum_k g_k L_k \otimes A_k, \tag{6.17}$$

where L_k and A_k are eigenoperators of the system and ancilla Hamiltonians respectivelly, with opposite sign Bohr frequency: ω_k for L_k and $-\omega_k$ for A_k. This garantees that each quanta that leaves/enters the system has the same energy of the one that enters/leaves the ancilla, retaining

---

[1] A matrix with no diagonal elements is a hollow matrix

no energy in the interaction. Let us use this condition on Eq. (6.9), remembering that we have dropped its subscript:

$$
\begin{aligned}
\mathcal{D}[\rho_S] &= -\frac{1}{2}\mathrm{Tr_A}[\mathrm{V},[\mathrm{V},\rho]] = \sum_{\mathrm{kj}} -\frac{1}{2}\mathrm{g_k g_j Tr_A[L_k A_k, [L_j A_j, \rho_S \rho_A]]} \\
&= \sum_{kj} -\frac{1}{2} g_k g_j \mathrm{Tr\{L_k L_j \rho_S A_k A_j \rho_A - L_k \rho_S L_j A_k \rho_A A_j} \\
&- L_j \rho_S L_k A_j \rho_A A_k + \rho_S L_j L_k \rho_A A_j A_k\} \\
&= \sum_{kj} -\frac{1}{2} g_k g_j \{\langle A_k A_j\rangle L_k L_j \rho_S - \langle A_j A_k\rangle L_k \rho_S L_j - \langle A_k A_j\rangle L_j \rho_S L_k + \langle A_j A_k\rangle \rho_S L_j L_k\}, \quad (6.18)
\end{aligned}
$$

where the averages are taken with respect to ρ_A. Since we are only using diagonal ancillae, all averages with respect to $A_k A_j$ are 0, exept for $A_k^\dagger A_k$ and $A_k A_k^\dagger$. Thus, rearranging Eq. (6.18), we finally have the familiar dissipator:

$$
\mathcal{D}[\rho_S] = \sum_k \gamma_k^- D[L_k] + \gamma_k^+ D[L_k^\dagger]. \tag{6.19}
$$

Here, $\gamma_k^- = g_k^2 \langle A_k A_k^\dagger\rangle$ and $\gamma_k^+ = g_k^2\langle A_k^\dagger A_k\rangle$. This result is very powerful. We see that the Lindblad master equation can be derived from a very simple setup. Notwithstanding, this method allows us to choose the operators L_k, as long as they are the building blocks of a resonant interaction. Thus, one can easily write a master equation in the repeated interacions setup by choosing V and ρ_A, ignoring midway calculations.

As an example, consider that both the system and all the ancillae are qubits. The interaction V is a hopping interaction and the ancillae are thermal:

$$
V = g(\sigma_S^\dagger \sigma_A + \sigma_S \sigma_A^\dagger), \tag{6.20}
$$

$$
\rho_A = \begin{pmatrix} f & 0 \\ 0 & 1-f \end{pmatrix} \tag{6.21}
$$

Inserting these in Eq. (6.19), the dissipator becomes

$$
\begin{aligned}
\mathcal{D}[\rho_S] &= g^2\,\mathrm{tr}\{\sigma_A^\dagger \sigma_A \rho_A\} D[\sigma_S] + g^2\,\mathrm{tr}\{\sigma_A \sigma_A^\dagger \rho_A\} D[\sigma_S^\dagger] \quad (6.22) \\
&= g^2 f D[\sigma_S] + g^2(1-f) D[\sigma_S^\dagger]. \quad (6.23)
\end{aligned}
$$

This is the amplitude damping channel for finite temperature, and its steady state solution is $\rho_{ss} = \rho_A$, as expected. It is thus shown that in the continuum limit the collisional model thermalizes the system without any need for approximations.

During this work we have generalized the above procedure in the following sense: suppose that, instead of identical ancillae colliding with the system, identical strings of different ancillae are doing so. How would the system be affected? The answer is simple, nevertheless very interesting. As before, we carry on the calculations up to order τ, taking the continuum limit afterwards. Consider a string of m ancillae ρ_m, interacting with the system during time τ/m and V rescaled as $m/\sqrt{\tau}$. The the first and second collisions yield, from Eq. (6.15),

$$\rho_S' = \rho_S - i\frac{\tau}{m}[H_S, \rho_S] + \tau\mathcal{D}_1[\rho_S], \tag{6.24}$$

$$\rho_S'' = \rho_S' - i\frac{\tau}{m}[H_S, \rho_S'] + \tau\mathcal{D}_2[\rho_S'], \tag{6.25}$$

where $\mathcal{D}_m$ is the dissipator due to ρ_m. Substituting Eq. (6.24) inside Eq. (6.25),

$$\begin{aligned} \rho_S'' &= \rho_S - i\frac{\tau}{m}[H_S, \rho_S] + \tau\mathcal{D}_1[\rho_S] - i\frac{\tau}{m}[H_S, \rho_S] + \tau\mathcal{D}_2[\rho_S] \\ \rho_S'' &= \rho_S - i\frac{2\tau}{m}[H_S, \rho_S] + \tau\mathcal{D}_1[\rho_S] + \tau\mathcal{D}_2[\rho_S]. \end{aligned} \tag{6.26}$$

This pattern continues on for the remaing ancillae. Thus, after the entire string we have

$$\rho_S^{(m)} = \rho_S - i\tau[H_S, \rho_S] + \tau\sum_{j=1}^{m}\mathcal{D}_j[\rho_S], \tag{6.27}$$

where $\rho_S^{(m)}$ is the state of the system after the entire string had sequentially interacted with it. If we assume several strings will do the same and take the continuum limit, replacing ρ' with $\rho_S^{(m)}$, we retrieve

$$\dot{\rho}_S = -i[H_S, \rho_S] + \sum_{j=1}^{m}\mathcal{D}_m[\rho_S]. \tag{6.28}$$

Surprisingly, the effect of a string of ancillae is additive in the master equation. Each ancilla in the string represents a different bath in contact with the system, without interference effects. With two different thermal ancillae, for example, we could lead the system to a non-equilibrium steady state [32].

6.3 Thermodynamics

An important application of collisional models is their ability to give a clean thermodynamic description of quantum processes [21, 75]. The basic formalism consists of energy preserving interactions, which where covered in the last section, and ancillae prepared in thermal states:

$$[H_0, V] = 0 \tag{6.29}$$

$$\rho_A = \rho_A^{\text{th}}. \tag{6.30}$$

In this setup, one can extract the first and second laws of thermodynamics. As we will see, although these laws will be only approximate for general maps, they become exact in the continuum limit. Let us begin with Eq. (6.15) before the continuum limit $\tau \to 0$:

$$\rho_S' = \rho_S - i[H_S, \rho_S]\tau + \mathcal{D}[\rho_S]\tau. \tag{6.31}$$

The first law of thermodynamics describes energy conservation and defines what is heat and what is work. We consider that no work is done, since the global evolution is a time independent unitary: there is no external energy input or output. Thus, every energy that is transfered must be in the form of heat.:

$$\Delta E = -Q, \tag{6.32}$$

where $E := \mathrm{Tr}\{\mathrm{H_S}\rho_\mathrm{S}\}$ and $Q := \mathrm{Tr}\{\mathrm{H_A}\rho_\mathrm{A}^{\text{th'}}\} - \mathrm{Tr}\{\mathrm{H_A}\rho_\mathrm{A}^{\text{th}}\}$. This is the first law of thermodynamics. Notice that associating the energy change of the chain of incoming ancillae with heat endorses our view of the collisional model as a reservoir. Another compelling argument to call it heat is the nature of the energy balance for the system and ancilla:

$$\begin{aligned}\Delta E = E' - E = \mathrm{Tr}\{\mathrm{H_S}\rho_\mathrm{S}'\} - \mathrm{Tr}\{\mathrm{H_S}\rho_\mathrm{S}\} &= -\mathrm{i}\tau\mathrm{Tr}\{\mathrm{H_S}[\mathrm{H_S}, \rho_\mathrm{S}]\} + \tau\mathrm{Tr}\{\mathrm{H_S}\mathcal{D}[\rho_\mathrm{S}]\} \\ &= \tau\mathrm{Tr}\{\mathrm{H_S}\mathcal{D}[\rho_\mathrm{S}]\}, \end{aligned} \tag{6.33}$$

$$\begin{aligned} Q &= \mathrm{Tr}\{\mathrm{H_A}\rho_\mathrm{A}^{\text{th'}}\} - \mathrm{Tr}\{\mathrm{H_A}\rho_\mathrm{A}^{\text{th}}\} \\ &= -i\tau\mathrm{Tr}\{\mathrm{H_A}[\mathrm{H_A} + \mathrm{G_A}/\sqrt{\tau}, \rho_\mathrm{A}^{\text{th}}]\} + \tau\mathrm{Tr}\{\mathrm{H_A}\mathcal{D}_\mathrm{A}[\rho_\mathrm{A}^{\text{th}}]\} \\ &= \tau\mathrm{Tr}\{\mathrm{H_A}\mathcal{D}_\mathrm{A}[\rho_\mathrm{A}^{\text{th}}]\}, \end{aligned} \tag{6.34}$$

where we noticed in the last equality that the commutator composed of one diagonal matrix is always hollow, and thus its product with another diagonal matrix is traceless as we saw before.

We see here that the energy trade stems from the dissipator alone, as in Chapter 5.

The second law is more intricate. We need first a definition of entropy production that is compatible with the physiscs of our model. Then, we see whether or not it relates to the standard notion developed by Clausius. The definition of entropy producion is motivated as a measure of irreversibility. We have already related irreversibility with information loss. In the collisional model setup, where ancillae are thrown away after the interaction with the system, we can spot two mechanisms for information loss. The first one is associated with the correlations built between the system and the outgoing ancillae, which are not accessible. The information associated with it can be cast as the variation of mutual information $\Delta\mathcal{I}(S|A)$ between S and A. The second one regards the change of the ancillary state, as we cannot access it for the same reason. This is quantified as the relative entropy $S(\rho_A^{\text{th'}}\|\rho_A^{\text{th}})$. Thus, the entropy production for each collision is the sum of both contributions [76]:

$$\Sigma := \Delta\mathcal{I}(S|A) + S(\rho_A^{\text{th'}}\|\rho_A^{\text{th}}). \tag{6.35}$$

This form for the entropy production is valid for any collisional model as general as Eq. (6.1). However it has no operational meaning, for it depends on the state of the bath, which we do not have access to. It is desirable to cast the entropy production only in terms system quantities. Although this is not the case for every map [32, 77], it can be done for more restrictive maps. The thermal map (6.31) is one of those. First, let us calculate the mutual information $\Delta\mathcal{I}(S|A)$ using (2.16):

$$\Delta\mathcal{I}(S|A) = S'_S + S'_A - S'_{SA} - (S_S + S_A - S_{SA}) = \Delta S_S + \Delta S_A, \tag{6.36}$$

where S_S, S_A and S_{SA} are the entropies of the system, ancilla and joint system respectivelly. In the last equality, we used the fact that the global evolution is unitary and thus conserves entropy. Inserting this on Eq. (6.35) and using the relative entropy (2.7), we can write

$$\begin{aligned}
\Sigma &= \Delta S_S + S'_A - S_A + S(\rho_A^{\text{th'}}\|\rho_A^{\text{th}}) \\
&= \Delta S_S + -\text{Tr}\{\rho_{\text{A}}^{\text{th'}} \log \rho_{\text{A}}^{\text{th'}}\} + \text{Tr}\{\rho_{\text{A}}^{\text{th}} \log \rho_{\text{A}}^{\text{th}}\} - \text{Tr}\{\rho_{\text{A}}^{\text{th'}} \log \frac{\rho_{\text{A}}^{\text{th}}}{\rho_{\text{A}}^{\text{th'}}}\} \\
&= \Delta S_S + \text{Tr}\{(\rho_{\text{A}}^{\text{th}} - \rho_{\text{A}}^{\text{th'}}) \log \rho_{\text{A}}^{\text{th}}\}.
\end{aligned} \tag{6.37}$$

The first term already relates to the system only. The second one is elusive. Let us open it by remembering that

$$\rho_A^{\text{th}} \left| j \right\rangle = p_j \left| j \right\rangle, \tag{6.38}$$

$$p_j = \exp\{-\beta E_j\}/Z, \tag{6.39}$$

where Z is the partition function and E_j are the energy eigenstates of the ancilla Hamiltonian. Using map (6.16) for a thermal state, we have

$$\begin{aligned}
\mathrm{Tr}\{(\rho_{\mathrm{A}}^{\text{th}} - \rho_{\mathrm{A}}^{\text{th'}}) \log \rho_{\mathrm{A}}^{\text{th}}\} &= \sum_j \left\langle j \right| (\rho_A^{\text{th}} - \rho_A^{\text{th'}}) \log \rho_A^{\text{th}} \left| j \right\rangle = \sum_j p_j \log p_j - \log p_j \left\langle j \right| \rho_A^{\text{th'}} \left| j \right\rangle \\
&= -\tau \sum_j \log p_j (\left\langle j \right| - i[H_A + G_A/\sqrt{\tau}, \rho_A^{\text{th}}] \left| j \right\rangle + \left\langle j \right| \mathcal{D}_A[\rho_A^{\text{th}}] \left| j \right\rangle) \\
&= \beta\tau \sum_j (E_j + \log Z) \left\langle j \right| \mathcal{D}_A[\rho_A^{\text{th}}] \left| j \right\rangle = \beta\tau \mathrm{Tr}\{\mathrm{H}_{\mathrm{A}} \mathcal{D}_{\mathrm{A}}[\rho_{\mathrm{A}}^{\text{th}}]\} \\
&= \beta Q = -\beta \Delta E.
\end{aligned}$$

Summing both terms and defining the free energy as $F = E - S/\beta$, the entropy production reads

$$\Sigma = \Delta S_S + \beta Q = -\beta \Delta F_S. \tag{6.40}$$

This is the second law of thermodynamics, derived for the collisional model. It is only valid up to order τ. However, in the continuum limit, the rate equation for the second law and the association of Q with energy leakage rate through the dissipator are both exact:

$$\dot{Q} = -\mathrm{Tr}\{\mathrm{H}_{\mathrm{S}} \mathcal{D}[\rho_{\mathrm{S}}]\}, \tag{6.41}$$

$$\Pi = \dot{S}_S + \beta \dot{Q} = -\beta \dot{F}_S, \tag{6.42}$$

where

$$\dot{S}_S := \lim_{\tau \to 0} \frac{\Delta S_S}{\tau}, \tag{6.43}$$

$$\dot{Q} := \lim_{\tau \to 0} \frac{Q}{\tau}, \tag{6.44}$$

$$\Pi := \lim_{\tau \to 0} \frac{\Sigma}{\tau}. \tag{6.45}$$

We have successfully wrote the first and second laws of thermodynamics in terms of the system information alone in the collisional model. The results match the desired effects for a system in contact with a thermal reservoir in the weak coupling limit: they are the same not only from a dynamical standpoint, as shown in the last section, and from a thermodynamical one as well.

Naturally, this is extends to the multiple bath scenario [32]. The first and second laws become

$$\dot{E} = -\sum_{j=1}^{m} \dot{Q}_m, \tag{6.46}$$

$$\Pi = \dot{S}_S + \sum_{j=1}^{m} \beta \dot{Q}_m, \tag{6.47}$$

where $\dot{Q}_m = -\mathrm{Tr H_S \mathcal{D}_m [\rho_S]}$.

6.4 Weakly coherent collisional models

In the previous sections, we had only considered ancillary states that are diagonal in the system energy basis. In those cases, we could derive a Lindblad master equation where the system evolves according to its own Hamiltonian and a dissipator related to the interaction with the sequence of ancillae. However, what would happen if the incoming ancillae had coherence in the energy basis? To answer this, let us write Eqs. (6.6) and (6.14) again, slightly modified:

$$\frac{\rho_S' - \rho_S}{\tau} = -i[H_S + \frac{G}{\sqrt{\tau}}, \rho_S] + \mathcal{D}[\rho_S] + \mathcal{O}(\tau). \tag{6.48}$$

$$G = \mathrm{Tr_A\{V\rho_A\}} \tag{6.49}$$

Before, we have noticed that in the limit of $\tau \to 0$ the contribution from G explodes and hence one cannot write the map as a master equation. By imposing a diagonal form for ρ_A, the divergence vanishes since that would make G trivially 0. In this section we propose a non-trivial alternative to the divergence of G.

We begin by defining the weakly coherent states

$$\rho_A = \rho_A^{\mathrm{th}} + \lambda \sqrt{\tau} \chi, \tag{6.50}$$

where χ is a hollow operator and λ represents a time scale and $\rho_A^{\text{th}} = \exp\{-\beta H_A\}/Z_A$ is a thermal state of inverse temperature β and partition function Z_A. Regard λ as a necessery quantity to keep χ in the same units as ρ_A^{th}. This is a thermal state with coherences, where all of them are incorporated inside χ. The diagonal state is considered to be thermal so that we can still draw a thermodynamical analysis out of it,but aside from this it would be no limitation to let its diagonal distribution be athermal.

Notice that the coherences in Eq. (6.50) are not arbitrary: they are proportional to the interaction time. In particular, in the continuum limit they become vanishingly small. Since this is the limit we are interested in, the name given to this class of states is justified. In general, not all states of the form (6.50) are positive semidefinite, but as $\tau \to 0$ this is ensured as long as the thermal state is not pure, i.e. the vacuum state, a condition that will be assumed from here on.

6.4.1 Hamiltonian engineering

Using the definition for G and remembering that $\mathrm{Tr_A}\{\mathrm{V}\rho_{\mathrm{A}}^{\mathrm{th}}\} = 0$, we see that ρ_A rescales $G \to \lambda\sqrt{\tau}G$. Hence, the map for S becomes

$$\frac{\rho_S' - \rho_S}{\tau} = -i[H_S + \lambda G, \rho_S] + \mathcal{D}[\rho_S] + \mathcal{O}(\sqrt{\tau}). \tag{6.51}$$

The leading order becomes $\sqrt{\tau}$ because of new terms related to $-\frac{\lambda\sqrt{\tau}}{2}\mathrm{Tr_A}[\mathrm{V},[\mathrm{V},\rho_{\mathrm{A}}^{\mathrm{th}} \otimes \chi]]$ that appear or the dissipator. In the continuum limit they will decay, thus no change is expected in the dissipative part of the dynamics. The unitary part, on the other hand, is incremented with a new term:

$$\dot{\rho}_S = -i[H_S + \lambda G, \rho_S] + \mathcal{D}[\rho_S], \tag{6.52}$$

$$G = \mathrm{Tr_A}\{\mathrm{V}\chi\}, \tag{6.53}$$

where G was redefined for simplicity. For concreteness, it is interesting to cast G in terms of eigenoperators as done with the dissipator in Eq. (6.19):

$$G = \mathrm{Tr_A}\{\mathrm{V}\chi\} = \sum_{\mathrm{i,j}} \langle \mathrm{i}|\, \mathrm{A_j} \otimes \mathrm{B_j}\, \chi\, |\mathrm{i}\rangle = \sum_{\mathrm{j}} \mathrm{A_j} \sum_{\mathrm{i}} \langle \mathrm{i}|\, \mathrm{B_j}\, \chi\, |\mathrm{i}\rangle = \sum_{\mathrm{j}} \langle \mathrm{B_j}\rangle_\chi \mathrm{A_j}, \tag{6.54}$$

where $\langle B_j\rangle_\chi = \mathrm{Tr}\{\mathrm{B_j}\ \chi\}$ is the average of the eigenoperators of the ancilla Hamiltonian with respect to its coherences. Thus, as a consequence of the structure of eigenoperators, we see that G is hollow in the system energy basis. The choice for its elements can be made through the interaction, and their relative intensities can be independently chosen from χ: with weak coherences, the collisional model can be used to perform Hamiltonian engineering.

For concreteness, consider the same example as in Section 6.2, but now the ancilla has a non-zero χ:

$$\chi = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{6.55}$$

The dissipator is the same, however there will be an additional term G

$$\begin{aligned} G &= g\,\mathrm{tr}\{\sigma_A^\dagger \chi\}\sigma_S + g\,\mathrm{tr}\{\sigma_A \chi\}\sigma_S^\dagger & (6.56) \\ &= g\sigma_x. & (6.57) \end{aligned}$$

The entire master equation will thus read

$$\dot{\rho_S} = -i[H_S + g\lambda\sigma_x] + g^2 f D[\sigma_S] + g^2(1-f)D[\sigma_S^\dagger]. \tag{6.58}$$

The presence of σ_x makes the steady state highly non-trivial and always coherent.

The additive property (6.28) shown for a sequence of different ancillae in thermal states is also valid when they are initialized in weakly coherent states. In the derivation, it was evident that the additive property stems from the fact that every cross term is of higher order in τ and thus disapears in the continuum limit. Since the single map structure of Eq. (6.51) is the same as the structure of Eq. (6.31), then for a string of m ancillas the master equation reads

$$\dot{\rho}_S = -i[H_S + \sum_{j=1}^{m} \lambda_j G_j, \rho_S] + \sum_{j=1}^{m} \mathcal{D}_j[\rho_S], \tag{6.59}$$

where the G_j are the Hamiltonians produced by each individual ancilla $\rho_A^{(j)}$.

6.4.2 Thermodynamics

We follow Section 6.3 closely, but always remarking the modifications induced by χ. The first law (6.32) stabilishes a relation between the energy leaving the system and the energy entering the bath. As the interaction still preserves energy, this should not change. However, the presence of an additional term in the Hamiltonian does play a role:

$$\dot{E}_S = d\langle H_S\rangle/dt = i\lambda\langle[G, H_S]\rangle + \text{tr}\{H_S\mathcal{D}[\rho_S]\}. \tag{6.60}$$

For detailed calculation, refer to Appendix A. The flux of energy entering the system now have two different contributions: one through a dissipator and another through a Hamiltonian. We argue here that, since the nature of the first one is dissipative, it is an incoherent source of energy just as heat. Nevertheless, the nature of the second source is unitarily coherent, just as work. We are thus inspired to define these rates as incoherent heat rate and coherent work rate:

$$\dot{\mathcal{W}}_C := i\lambda\langle[G, H_S]\rangle, \tag{6.61}$$

$$\dot{Q}_{inc} := \text{tr}\{H_S\mathcal{D}[\rho_S]\}, \tag{6.62}$$

$$\dot{E}_S = \dot{\mathcal{W}}_C + \dot{Q}_{inc}. \tag{6.63}$$

Quite surprisingly, we will shortly show that these quantities do behave as work and heat, respectively. If not for the coherences in ρ_A, all the energy that would be transfered to ρ_S would be dissipative. However, by means of G, a transformation process occurs and the bath coherently injects a fraction of its lost energy in the system. This is the statement of the first law.

For the second law, we must refer back to Eq. (6.35):

$$\Sigma = \Delta\mathcal{I}(S|A) + S(\rho'_A\|\rho_A). \tag{6.64}$$

The detailed calculations are done in Appendix B and C, and the results are exposed bellow:

$$\Delta\mathcal{I}(S|A) = -\beta\Delta F - \Delta C_{rel}(\rho_A), \tag{6.65}$$

$$S(\rho'_A\|\rho_A) = \beta\mathcal{W}_C + \Delta C_{rel}(\rho_A), \tag{6.66}$$

where $F := E - TS(\rho_S)$ is the system free energy, $T = \beta^{-1}$ is the temperature and $\mathcal{W}_C \simeq \dot{\mathcal{W}}_C\tau$ is the approximate coherent work done in a single collision. Summing over both contributions and once again taking the continuum limit $\tau \to 0$, we finnaly write

$$\Pi = \beta(\dot{\mathcal{W}}_C - \dot{F}) = \dot{S}_S - \beta\dot{Q}_{inc} \geq 0. \tag{6.67}$$

This equation is a direct analog of the usual second law of thermodynamics. One should notice here that both incoherent heat and coherent work play the usual roles inside the functional form of the entropy production. This once again motivates our terminology, where heat is associated with the Clausius formulation of entropy and work follows the famous inequality

$$\dot{\mathcal{W}}_C \geq \dot{F}. \tag{6.68}$$

Thus, the amount of work done in the system is bounded by the free energy difference experienced by the system.

The structure of Eq. (6.59) signals at a straightforward extention of both the first and second law to multiple reservoirs. Since the coherent work and incoherent heat depend on the ancillae because of G and $\mathcal{D}$ alone, then the noninterference between G_j and $\mathcal{D}_j$ of each ancilla results on

$$\dot{E}_S = \sum_{j=1}^{m} \left\{ \dot{\mathcal{W}}_C^{(j)} + \dot{Q}_{inc}^{(j)} \right\} \tag{6.69}$$

$$\Pi = \dot{S}_S - \sum_{j=1}^{m} \beta_j \dot{Q}_{inc}^{(j)}. \tag{6.70}$$

6.4.3 Resource interconversion

Before proceeding to the conclusion of this work, we put forth the main finding of this work. Although Eq. (6.68) provides a bound for work done or received by the system, Eq. (6.66) and Eq. (6.65) offer a much more interesting one. Directly from Eq. (6.66), we can use the positivity of the relative entropy shown in Chapter 2 to write

$$\mathcal{W}_C \geq -T\Delta C_{rel}(\rho_A). \tag{6.71}$$

This offers a second bound on work extraction which is tighter than Eq. (6.68), as can be seen from Eq. (6.65):

$$-T\Delta C_{rel}(\rho_A) = T\Delta\mathcal{I}(S|A) + \Delta F \geq \Delta. \tag{6.72}$$

The last inequality relies on $\Delta\mathcal{I}(S|A) \geq 0$, which is quite intuitive since the amount of correlations before the interaction is 0.

This result stabilishes a bridge between genuinelly quantum resources and a classical resource such as work. Here, the variation of coherences in the bath allow for the transformation process of the incoherent energy contained inside it into coherent energy injection in the system. From Eq. (6.61), it is evident that if $\lambda = 0$, i.e. there are no coherences in the bath, there is no work available for the system, corroborating with the view that the coherences not only bound the work done, but are essencial for its existence.

As a final remark, bound (6.68) is only put in terms of system quantities, while bound (6.71) makes explicit reference to the bath. This is a signature of the athermality of the bath modeled by the weakly coherent ancillae, where the tightest bound cannot wriggle out of a refecence to the bath. This discussion is made on reference [77], where the tighter bound is actually the same as ours.

Chapter 7

Conclusions

In this dissertation we have introduce quantum information and open quantum systems tools to develop the theory of collisional models. We have shown that such setup provides a clean platform to model and probe a reservoir. Through it, no approximation is needed to achieve the GKSL equation and its free parameters are all related to quantities that are in principle controlable in the laboratory, such as the state of the ancillae and the interaction they experience with the system of interest [78, 79]. Furthermore, we have shown that the repetitive use of different ancillae have an additive effect over the dissipators of the GKSL equation, so that the local approximation for master equations is exact, in opposition to real environments [80]. With the aid of information-theoretic tools, we have also explicitly derived thermodynamic relations out of this model for thermal ancillae, which give rise to the same laws as system weakly coupled to a thermal bath. As a novelty, we propose a new class of states that hold great proximity to thermal states, but yielding a small amount of coherences: the weakly coherent states. We show that not only ancillae initialized in these states also provide a differential equation to the local evolution of the system, but that this evolution is the same as a weakly coupled thermal bath alongside unitary driving. This setup is also extendable to a string of different ancillae, with the same additive property. Surprisingly, despite the modeled environment not being thermal, the system is still governed by the first and second laws of thermodynamics, equiped with peculiar modifications. In the first law, a work-like term appears albeit the evolution of the global system being time independent. In the second law, a tighter version for this work-like quantity extraction can be related to the change of coherences quantified by the variation of relative entropy of coherence in the ancillae. This provides a bridge between quantum resources, i.e. coherences, and a thermal resource such as work. It also shows that the law of thermodynamics are not restricted to thermal reservoirs, as was already shown for squeezed states [15].

There are several possible paths for future research. The derivation for the GKSL equation using the collisional model relied on the fact that the interactions were all in sequence, with the same interaction time. However, this pressuposes that one has perfect control over the incoming ancillae, which is not true for a real reservoir. To adress such baths, one can set the arrival time of the ancillae as a Poisson process [21]. Furthermore, using the multiple bath formalism developed here, it should be interesting to understand how the weak coherences affect heat transport between reservoirs [81], and if it is possible to define a coherence current between them. This should prove useful as a form of coherence transfer from systems that one has good control over to other that one has not. Finnaly, it should prove interesting to relate our findings to ergotropy of the initial state of the ancillary systems, as they are initially in an active state (athermal) and thus can have work extracted from them [82].

Appendix A

Changes in the ancilla

In this appendix we provide the updated state of the ancillae, after they have interacted with the system. This can be obtained by taking the partial trace of Eq. (6.5) over S, in a calculation analogous to the one that led to Eq. (6.10). First, let us rewrite the global map in a useful way:

$$\rho'_{SA} = \rho_S\rho_A - i\tau[H_{SA},\rho_S\rho_A] - \frac{\tau^2}{2}[H_{SA},[H_{SA},\rho_S\rho_A]]. \tag{A.1}$$

Taking the partial trace with respect to S, we have

$$\rho'_A = \rho_A^{\text{th}} + \sqrt{\tau}\Big(\lambda\chi_A - i[G_A,\rho_A^{\text{th}}]\Big) + \tau\Big(-i\lambda[G_A,\chi_A] + D_A(\rho_A^{\text{th}})\Big). \tag{A.2}$$

where

$$G_A = \text{tr}_S(V_{SA}\rho_S), \tag{A.3}$$

$$D_A(\rho_A^{\text{th}}) = -\frac{1}{2}\,\text{tr}_S[V_{SA},[V_{SA},\rho_S\rho_A^{\text{th}}]]. \tag{A.4}$$

Quite relevant to the discussion below, the term of order $\sqrt{\tau}$ does not vanish in Eq (A.2), since there is no restriction to the amount of coherence ρ_S has.

A.1 Energy balance

Using the general map (A.1) we can compute the changes in energy of the system and ancilla, defined as $\Delta H_S = \operatorname{tr}\{H_S(\rho'_{SA} - \rho_S\rho_A)\}$ and $\Delta H_A = \operatorname{tr}\{H_A(\rho'_{SA} - \rho_S\rho_A)\}$. One then readily finds

$$\Delta H_S = i\sqrt{\tau}\langle[V_{SA}, H_S]\rangle_{SA} + \frac{\tau}{2}\langle[V_{SA}, [V_{SA}, H_S]]\rangle_{SA}, \tag{A.5}$$

$$\Delta H_A = i\sqrt{\tau}\langle[V_{SA}, H_A]\rangle_{SA} + \frac{\tau}{2}\langle[V_{SA}, [V_{SA}, H_A]]\rangle_{SA}. \tag{A.6}$$

where $\langle\ldots\rangle_{SA}$ means averages over $\rho_S\rho_A$. Notice that the structure of these results is entirely independent on any specific choice for the states of the ancillae. Due to strong energy conservation, $[V_{SA}, H_S + H_A] = 0$ it follows that

$$\langle[V_{SA}, H_S]\rangle_{SA} = -\langle[V_{SA}, H_A]\rangle_{SA}, \tag{A.7}$$

$$\langle[V_{SA}, [V_{SA}, H_S]]\rangle_{SA} = -\langle[V_{SA}, [V_{SA}, H_A]]\rangle_{SA}, \tag{A.8}$$

and hence

$$\Delta H_S = -\Delta H_A. \tag{A.9}$$

Two conclusions may be drawn from this. The first is that, as mentioned in the main text, the strong energy conservation condition (4) implies that no work is performed; all change in energy in the system stems from a corresponding change in the ancillae. Second, Eqs. (A.7) and (A.8) allow us to pinpoint the origin of the coherent work $\mathcal{W}_C$ and the incoherent heat $\mathcal{Q}_{\text{inc}}$ appearing in Eq. (6.63) of the main text.

To accomplish this, we simply need to express global averages over $\rho_S\rho_A$ in terms of local averages over either ρ_S or ρ_A. For instance, referring to Eq. (A.5), the first term is precisely the coherent work since

$$\mathcal{W}_C = i\lambda\tau\langle[G, H_S]\rangle_S = i\sqrt{\tau}\langle[V_{SA}, H_S]\rangle_{SA}.$$

The identity in Eq. (A.7) therefore implies that this contribution will stems from a corresponding term on the side of the ancilla of the form $\langle[V_{SA}, H_A]\rangle$. Whence,

$$\mathcal{W}_C = -i\sqrt{\tau}\langle[V_{SA}, H_A]\rangle_{SA} = -i\sqrt{\tau}\langle[G_A, H_A]\rangle_A, \tag{A.10}$$

where G_A is given in Eq. (A.3). In the last term, the average over ρ_A^{th} does not contribute, so we finally get

$$\mathcal{W}_C = -i\lambda\tau\langle[G_A, H_A]\rangle_{\chi_A}. \tag{A.11}$$

Similarly, the incoherent heat $\mathcal{Q}_{\text{inc}}$ is related to the second term in Eq. (A.5):

$$\mathcal{Q}_{\text{inc}} = \tau\,\text{tr}\left\{H_S D(\rho_S)\right\} = \frac{\tau}{2}\langle[V_{SA}, [V_{SA}, H_S]]\rangle = -\frac{\tau}{2}\langle[V_{SA}, [V_{SA}, H_A]]\rangle = -\tau\,\text{tr}\left\{H_A D_A(\rho_A^{\text{th}})\right\}, \tag{A.12}$$

where $D_A(\rho_A^{\text{th}}) = -\frac{1}{2}\,\text{tr}_S[V_{SA}, [V_{SA}, \rho_S\rho_A^{\text{th}}]]$. The total change in energy of the system, which is the heat leaving the ancilla, can then be written solely in terms of ancilla-based quantities:

$$\Delta\langle H_S\rangle := -Q_A = \mathcal{W}_C + \mathcal{Q}_{\text{inc}} = -i\lambda\tau\langle[G_A, H_A]\rangle_{\chi_A} - \tau\,\text{tr}\left\{H_A D_A(\rho_A^{\text{th}})\right\}. \tag{A.13}$$

These results therefore allow us to pinpoint which terms in the heat ΔH_A leaving the ancilla are converted to $\mathcal{W}_C$ and $\mathcal{Q}_{\text{inc}}$.

Appendix B

Series expansions

The states of system and ancilla, before and after the interactions, will generally depend on τ in different ways. To compute the entropy production, defined in Eq. (6.35) of the main text, one must compute several entropic quantities depending on these states. Since we are interested in the limit $\tau \to 0$, these quantities can be computed using perturbation theory, which becomes exact in the limit $\tau \to 0$. We start by stating some general results on perturbative expansions of the von Neumann entropy, the relative entropy of coherence and the quantum Kullback-Leibler divergence (relative entropy).

B.1 Von Neumann entropy

Consider a general density matrix of the form

$$\rho = \rho_0 + \epsilon\sigma, \tag{B.1}$$

where ϵ is a small parameter and we assume $\operatorname{tr}\rho_0 = 1$ so $\operatorname{tr}\sigma = 0$. Let $\rho_0 = \sum_i p_i |i\rangle\langle i|$ denote the eigendecomposition of the unperturbed density matrix ρ_0. We now wish to compute the von Neumann entropy of ρ, which reads

$$S(\rho) = -\operatorname{tr}(\rho\log\rho) = -\sum_i P_i \log P_i, \tag{B.2}$$

where P_i are the eigenvalues of the full density matrix ρ.

Since ρ is a Hermitian operator, standard perturbation theory applies [83]. Assuming that the p_i are non-degenerate, we may then write, up to order ϵ^2,

$$P_i = p_i + \epsilon\sigma_{ii} + \epsilon^2 \sum_{j\neq i} \frac{|\sigma_{ij}|^2}{p_i - p_j}. \tag{B.3}$$

Plugging this in Eq. (B.2), expanding $P_i \log P_i$ in ϵ up to second order and using the fact that $\operatorname{tr}\sigma = 0$, we find that

$$S(\rho) = S(\rho_0) - \epsilon \sum_i \sigma_{ii} \log p_i - \epsilon^2 \sum_i \left\{ \frac{\sigma_{ii}^2}{2p_i} + \sum_{j\neq i} \frac{|\sigma_{ij}|^2}{p_i - p_j} \log p_i \right\}. \tag{B.4}$$

This is the series expansion for $S(\rho)$. The populations σ_{ii} contribute both with order ϵ and ϵ^2, whereas the coherences (off-diagonals) only start to contribute at order ϵ^2.

B.2 Relative entropy of coherence

Due to this separation, the relative entropy of coherence [Eq. (19) of the main text] will be of order ϵ^2:

$$C(\rho) = \epsilon^2 \sum_{i,j\neq i} \frac{|\sigma_{ij}|^2}{p_i - p_j} \log p_i. \tag{B.5}$$

This expression can also be written more symmetrically, as

$$C(\rho) = \frac{\epsilon^2}{2} \sum_{i,j\neq i} \frac{|\sigma_{ij}|^2}{p_i - p_j} \log p_i/p_j. \tag{B.6}$$

Thus, we see that the relative entropy of coherence weights each coherence $|\sigma_{ij}|$ by a factor of the form

$$\frac{\log(x/y)}{x-y} \geq 1, \qquad x, y \in [0,1].$$

B.3 Quantum relative entropy

Next we consider the relative entropy $S(\rho'\|\rho)$ between two density matrices of the form

$$\rho = \rho_0 + \epsilon\sigma, \qquad \rho' = \rho_0 + \epsilon\mu, \tag{B.7}$$

where σ and μ are arbitrary, but both depend on ρ_0 to order ϵ^0. We have

$$S(\rho' \| \rho) = -S(\rho') - \operatorname{tr}(\rho' \log \rho). \tag{B.8}$$

The first term was already found in (B.4), with σ replaced by μ:

$$S(\rho') = S(\rho_0) - \epsilon \sum_i \mu_{ii} \log p_i - \epsilon^2 \sum_i \left\{ \frac{\mu_{ii}^2}{2p_i} + \sum_{j \neq i} \frac{|\mu_{ij}|^2}{p_i - p_j} \log p_i \right\}. \tag{B.9}$$

In order to compute the last term we will need not only the perturbation theory for the eigenvalues of ρ [Eq. (B.3)], but also for its eigenvectors. Defining $\rho = \sum_i P_i |\tilde{i}\rangle\langle\tilde{i}|$ allows us to write

$$\operatorname{tr}(\rho' \log \rho) = \sum_i \langle \tilde{i} | \rho' | \tilde{i} \rangle \log P_i. \tag{B.10}$$

Thus, in addition to writing $\log P_i$ as a power series, we will also have to expand $\langle \tilde{i} | \rho' | \tilde{i} \rangle$.

Using standard perturbation theory, the eigenvectors of ρ can be written as

$$|\tilde{i}\rangle = |i\rangle + \epsilon |i_1\rangle + \epsilon^2 |i_2\rangle, \tag{B.11}$$

where

$$|i_1\rangle = \sum_{j \neq i} |j\rangle \frac{\sigma_{ij}}{p_i - p_j}, \tag{B.12}$$

$$|i_2\rangle = -\frac{1}{2}|i\rangle \sum_{j \neq i} \frac{|\sigma_{ij}|^2}{(p_i - p_j)^2} - \sum_{j \neq i} |j\rangle \frac{\sigma_{ii}\sigma_{ji}}{(p_i - p_j)^2} + \sum_{j \neq i, k \neq i} |k\rangle \frac{\sigma_{kj}\sigma_{ji}}{(p_i - p_j)(p_i - p_k)} \tag{B.13}$$

With this we find, after carrying out the computations,

$$\langle \tilde{i} | \rho' | \tilde{i} \rangle = p_i + \epsilon \mu_{ii} + \epsilon^2 \sum_{j \neq i} \frac{\mu_{ij}\sigma_{ji} + \sigma_{ij}\mu_{ji} - |\sigma_{ij}|^2}{p_i - p_j}. \tag{B.14}$$

Plugging this result in Eq. (B.10) and expanding all terms in ϵ then finally leads to

$$\operatorname{tr}(\rho' \log \rho) = \sum_i \left\{ p_i \log p_i + \epsilon(\sigma_{ii} + \mu_{ii} \log p_i) + \epsilon^2 \left[\frac{\mu_{ii}\sigma_{ii}}{p_i} - \frac{\sigma_{ii}^2}{2p_i} + \sum_{j \neq i} \frac{\mu_{ij}\sigma_{ji} + \sigma_{ij}\mu_{ji} - |\sigma_{ij}|^2}{p_i - p_j} \log p_i \right] \right\}. \tag{B.15}$$

Finally, combining this with Eq. (B.9) leads to

$$S(\rho'\|\rho) = \frac{\epsilon^2}{2}\sum_i \left\{ \frac{(\mu_{ii} - \sigma_{ii})^2}{p_i} + \sum_{j\neq i} \frac{|\mu_{ij} - \sigma_{ij}|^2}{p_i - p_j} \log(p_i/p_j) \right\}. \tag{B.16}$$

We therefore see that while $S(\rho)$ and $S(\rho')$ contain contributions of order ϵ, the first non-zero contribution to the relative entropy is of order ϵ^2. Moreover, the result depends on both the populations and the coherences, and both with the same order ϵ^2. This highlights some of the differences between $S(\rho'\|\rho)$ and $S(\rho') - S(\rho)$.

Appendix C

Entropy production series expansion

We are now in the position to derive Eqs. (6.65) and (6.66) of the main text. To do so, one must simply apply the results of Sec. S2 with the appropriate choices of ρ, ρ_0, etc. Since system and environment always start uncorrelated and since the global dynamics is unitary, the mutual information developed in the map (A.1) can be written as

$$\mathcal{I}(\rho'_{SA}) = S(\rho'_S) + S(\rho'_A) - S(\rho'_{SA}) := \Delta S_S + \Delta S_A. \tag{C.1}$$

Our task is to compute $\Delta S_A = S(\rho'_A) - S(\rho_A)$. In addition, we will also need $S(\rho'_A \| \rho_A)$. We compute each term separately.

C.1 Calculation of $S(\rho_A)$

The initial state of the ancilla is given in Eq. (6.50) of the main text, $\rho_A = \rho_A^{\text{th}} + \sqrt{\tau}\lambda\chi_A$, where χ_A has no diagonal elements. This falls under the structure of Eq. (B.1), provided we identify

$$\epsilon\sigma = \sqrt{\tau}\lambda\chi_A.$$

A direct application of Eq. (B.4) then yields

$$S(\rho_A) = S(\rho_A^{\text{th}}) - \lambda^2\tau \sum_{i,j\neq i} \frac{|(\chi_A)_{ij}|^2}{p_i^{\text{th}} - p_j^{\text{th}}} \log p_i^{\text{th}}, \tag{C.2}$$

where p_i^{th} are the eigenvalues of ρ_A^{th} and the basis $|i\rangle$ refers to the energy basis of H_A. Since the perturbed part of ρ_A has no diagonal elements, the second term in Eq. (C.2) is nothing but the relative entropy of coherence of the state ρ_A,

$$C(\rho_A) = \lambda^2 \tau \sum_{i,j\neq i} \frac{|(\chi_A)_{ij}|^2}{p_i^{\text{th}} - p_j^{\text{th}}} \log p_i^{\text{th}}. \tag{C.3}$$

Thus, we may simply write

$$S(\rho_A) = S(\rho_A^{\text{th}}) - C(\rho_A). \tag{C.4}$$

C.2 Calculation of $S(\rho'_A)$

The state of the ancilla after the map is given by Eq. (A.2). This once again has the structure Eq. (B.1), but now one must identify

$$\epsilon\sigma = \sqrt{\tau}\Big\{\lambda\chi_A - i[G_A, \rho_A^{\text{th}}]\Big\} + \tau\Big\{-i\lambda[G_A, \chi_A] + D_A(\rho_A^{\text{th}})\Big\}$$

The terms proportional to $\sqrt{\tau}$ now form the off-diagonal part of σ and those proportional to τ are all diagonal. Applying again Eq. (B.4) yields

$$S(\rho'_A) = S(\rho_A^{\text{th}}) - \tau \sum_i \Big(-i\lambda[G_A, \chi_A] + D_A(\rho_A^{\text{th}})\Big)_{ii} \log p_i^{\text{th}} - \tau \sum_{i,j\neq i} \frac{\Big|\Big(\lambda\chi_A - i[G_A, \rho_A^{\text{th}}]\Big)_{ij}\Big|^2}{p_i^{\text{th}} - p_j^{\text{th}}} \log p_i^{\text{th}}.$$

Once again, comparing with Eqs. (B.4) and (B.5), the relative entropy of coherence of ρ'_A corresponds to the last term only,

$$C(\rho'_A) = \tau \sum_{i,j\neq i} \frac{\Big|\Big(\lambda\chi_A - i[G_A, \rho_A^{\text{th}}]\Big)_{ij}\Big|^2}{p_i^{\text{th}} - p_j^{\text{th}}} \log p_i^{\text{th}}. \tag{C.5}$$

That is, we may write

$$S(\rho'_A) = S(\rho_A^{\text{th}}) - \tau \sum_i \Big(-i\lambda[G_A, \chi_A] + D_A(\rho_A^{\text{th}})\Big)_{ii} \log p_i^{\text{th}} - C(\rho'_A).$$

The term proportional to τ, on the other hand, can be written as

$$-\tau \sum_i \Big(-i\lambda[G_A, \chi_A] + D_A(\rho_A^{\text{th}})\Big)_{ii} \log p_i^{\text{th}} = \beta\tau\, \text{tr}_A \Big\{\Big(-i\lambda[G_A, \chi_A] + D_A(\rho_A^{\text{th}})\Big)H_A\Big\}$$

where we also use the fact that $\log \rho_A^{\text{th}} = -\beta H_A - \log Z_A$ [c.f. Eq. (6.50) of the main text]. The term proportional to $\log Z_A$ vanishes, for it is proportional to $\text{tr}(\rho_A' - \rho_A)$, and the second is therefore nothing but the total change in energy of the ancilla in Eq. (A.13). But this, in turn, is minus the change in energy in the system. Whence, we conclude that

$$S(\rho_A') = S(\rho_A^{\text{th}}) - \beta\Delta\langle H_S\rangle - C(\rho_A'). \tag{C.6}$$

C.3 Calculation of $\mathcal{I}(\rho_{SA}')$

Inserting Eqs. (C.4) and (C.6) into Eq. (C.1) leads to

$$\mathcal{I}(\rho_{SA}') = \Delta S_S - \beta\Delta\langle H_S\rangle - \Delta C_A, \tag{C.7}$$

which is Eq. (6.65) of the main text, provided we recognize $\Delta S_S - \beta\Delta\langle H_S\rangle = -\beta\Delta F$, as the change in free energy of the system.

C.4 Calculation of $S(\rho_A'\|\rho_A)$

Finally, we turn to the relative entropy $S(\rho_A'\|\rho_A)$, expressed as the series in Eq. (B.16). The operators μ and σ, defined in Eq. (B.7), should now be recognized with

$$\begin{aligned}
\epsilon\sigma &= \sqrt{\tau}\lambda\chi_A, \\
\epsilon\mu &= \sqrt{\tau}\Big\{\lambda\chi_A - i[G_A, \rho_A^{\text{th}}]\Big\} + \tau\Big\{ - i\lambda[G_A, \chi_A] + D_A(\rho_A^{\text{th}})\Big\}.
\end{aligned}$$

The first term in Eq. (B.16) will depend only on the diagonal part of μ (the diagonal part of σ is zero). But this term is already of order τ, so this will ultimately lead to a contribution of order τ^2.

The only non-negligible term is thus the one related to the coherences. It is convenient to express $|\mu_{ij} - \sigma_{ij}|^2$ as

$$|\mu_{ij} - \sigma_{ij}|^2 = |\mu_{ij}|^2 - |\sigma_{ij}|^2 + \Big(2|\sigma_{ij}|^2 - \mu_{ij}\sigma_{ji} - \sigma_{ij}\mu_{ji}\Big).$$

The reason why this is useful is because then the first two terms can be recognized as the difference between the relative entropies of coherence of ρ'_A and ρ_A respectively [Eqs. (C.5) and (C.3)]. On the other hand, the remaining term in parendissertation may be written as

$$2|\sigma_{ij}|^2 - \mu_{ij}\sigma_{ji} - \sigma_{ij}\mu_{ji} = i\lambda\Big[(\chi_A)_{ij}(G_A)_{ji} - (G_A)_{ij}(\chi_A)_{ji}\Big](p_i^{\mathrm{th}} - p_j^{\mathrm{th}}).$$

Substituting these results in Eq. (B.16) and expressing the remaining summations in terms of a trace, then yields

$$S(\rho'_A \| \rho_A) = \Delta C_A - i\lambda\beta\tau\langle[G_A, H_A]\rangle_{\chi_A}.$$

Comparing this with Eq. (A.11), we finally arrive at Eq. (6.66) of the main text; viz.,

$$S(\rho'_A \| \rho_A) = \Delta C_A + \beta\mathcal{W}_C. \tag{C.8}$$

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