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STOCHASTIC THERMODYNAMICS FOR OPEN QUANTUM SYSTEMS IN THE
REPEATED INTERACTION SCHEME

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Usamos la teoría de termodinámica estocástica para estudiar sistemas cuánticos cuya dinámica es descrita por mapas completamente positivos que preservan la traza (CPTP en inglés) debido a su interacción con un baño térmico. Estudiamos una clase más amplia de mapas con equilibrio, entre los cuales los mapas termales son solo un caso especial. En general, para mapas CPTP las cantidades termodinámicas tales como la producción de entropía y el trabajo realizado sobre el sistema dependen del estado combinado del sistema más baño. Mostramos que para mapas con equilibrio estas cantidades pueden ser escritas en términos de propiedades del sistema únicamente. Las relaciones que obtenemos son válidas para una intensidad de acoplamiento arbitraria entre el sistema y el baño termal. Estudiamos las fluctuaciones de las cantidades termodinámicas en el esquema de medición de dos puntos. Derivamos teoremas de fluctuación detallados para la producción de entropía y el trabajo y obtenemos algunas simplificaciones para el caso de los mapas con equilibrio. Ilustramos nuestros resultados considerando un espín en un ciclo termodinámico y una cadena de espines $1/2$ acopladas a un baño por uno de sus bordes. Conectamos además la condición de balance detallado cuántico para ecuaciones maestras de Lindblad con la propiedad de equilibrio de los mapas CPTP que, al iterarlos y en un límite particular, generan la ecuación maestra. Mostramos cómo obtener una concatenación de mapas que genera una ecuación de Lindblad forzada por los bordes dada a priori, como una forma de construir una termodinámica consistente para la dinámica de Lindblad.

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We use the theory of stochastic thermodynamics to study quantum systems whose dynamics are described by completely positive trace preserving (CPTP) maps due to its interaction with a thermal bath. We study a broader class of equilibrium maps, of which thermal maps are just a special case. These have an invariant state for which the entropy production vanishes when they act over these states. In general, for CPTP maps the thermodynamic quantities such as entropy production or work performed on the system depend on the combined state of the system plus its environment. We show that these quantities can be written in terms of system properties for equilibrium maps. The relations we obtain are valid for arbitrary strength coupling between the system and thermal bath. We study the fluctuations of thermodynamic quantities in a two-point measurement scheme. We derive detailed fluctuation theorems for the entropy production and work and obtain some simplifications for equilibrium maps. We illustrate our results considering a single spin in a thermodynamic cycle and a spin $1/2$ chain coupled to a bath by one of its boundaries. We further connect the condition of quantum detailed balance for Lindblad master equations to the equilibrium property of CPTP maps that when iterated and in a particular limit generates the master equation. We show how to obtain a concatenation of CPTP maps that generates an a priori given boundary driven Lindblad equation as a way to construct a consistent thermodynamic framework for the Lindblad dynamics.

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Introduction

In the last decades experiments have been dealing with increasingly smaller systems in which thermal and quantum fluctuations play a major role, thus it is necessary a thermodynamic description that is capable of dealing with far from equilibrium systems and at the same time account for non-classical features.

The theory of stochastic thermodynamics has been increasingly useful in describing far from equilibrium processes. It studies the relations between energy, heat, work and entropy at small scales in systems driven arbitrarily far from equilibrium. In the past decades it has had an important development mainly due to the discovery of the integral and detailed fluctuation theorems for work and entropy production [1, 2, 3, 4]. The integral fluctuation theorem is a consequence of the detailed fluctuation theorem, which relates the probabilities of creating and annihilating a certain amount of entropy or producing and dissipating a certain amount of work in processes which can be far from equilibrium. In the early beginnings the theory draw the interest of the people due to its ability to obtain equilibrium thermodynamic quantities even when the system one is studying is far from equilibrium. But now, because It is even possible to derive from it the second law of thermodynamics for a system in contact with a thermal bath, some suggest to consider it stronger and more fundamental than the second law itself. These theorems have been vastly verified in a variety of contexts: numerical simulations, polymers, biomolecules like RNA or DNA, protein folding, colloidal particles driven by time-dependent lasers, etc. [4, 5, 6, 7]. Later works have extended these relations to quantum dynamics [8, 9, 10] and they have also been verified in the laboratory in this context [11, 12].

For many systems of interest, the coupling energy between the system and bath can be neglected in comparison with their energies. In this case, a thermodynamic framework normally referred to as "in the weak coupling" is very successful. In particular, work is performed in the system by externally modifying a control parameter of the system Hamiltonian, for instance by changing a field that varies the system energy levels. In this case, from the stochastic thermodynamics quantities, which are defined in terms of trajectories (in phase space for classical dynamics and in the space of measurement outcomes in quantum dynamics), one can recover the ensemble thermodynamics quantities of [13, 14, 15]. These quantities are local in the sense that they can be written in terms of variables of the system of interest, without needing knowledge of the bath besides its temperature.

There are other systems of interest which cannot be described as driven system weakly coupled to a thermal bath. Among other reasons this might be because the baths are prepared

in non-equilibrium states, there is information processing which must be taken into account like in the various examples of “Maxwell demons”, or the coupling is controlled in an active way. The later has been studied in [16], where a quantum system interacts sequentially with many identical copies of an external probe by its boundaries. In this work, we have in mind such a setup and with the purpose of studying thermodynamic processes, we consider the simple situation in which the external probe is prepared in a thermal state. Thus we shall refer to the probe as the bath, even though we are not assuming it is macroscopic. The experimenter controls the coupling at some work cost, and a certain amount of heat will also flow between the system and the bath. These thermodynamic quantities are in this case completely determined by the coupling energy. An appropriate formalism to analyse these quantum evolutions and the thermodynamic behavior is that of *completely positive trace preserving* (CPTP) maps [17]. In particular, one would like to account for the coupling between the system and the bath non-perturbatively. The thermodynamic properties of systems strongly coupled to a bath are not yet well understood although they have been considered in [18, 19, 20, 21].

We study the quantum stochastic thermodynamics of CPTP maps as formulated in [18, 22, 23, 24] where one considers that the system plus environment evolve unitarily during the process from an uncorrelated initial state and therefore the change in the system due to this process is given by a CPTP map. In this formulation, the strength of the coupling is arbitrary and thus the thermodynamic quantities such as the work performed on the system, the total heat exchange between the system and the bath and the total entropy production are *non-local* quantities, this means, they are expressed in terms of the total system-bath density matrix at the beginning and end of the process. In the limit where the strength of the coupling vanishes one recovers the expressions obtained in the weak coupling regime which are local, i.e., they depend only on system’s operators. In our study, we make use of the theory of stochastic thermodynamics through a two-point measurement scheme [25]. The thermodynamic quantities are defined for every stochastic trajectory in the outcome space of these measurements in such a way that upon averaging the standard definitions for the mean quantities are recovered. The fluctuation theorems for this repeated interaction scheme has been studied in [22, 24], where a system is driven by a time dependent protocol. Here we derive these relations but emphasize on a process where the system itself is not driven but the interaction with the bath is externally controlled.

A process may involve several interactions with a bath, each one described as a CPTP map, and thus a sequence of different maps may act on the system. In particular, repeating the same sequence may bring the system to a stationary or invariant state. In general, an invariant state of a CPTP map represents a *non-equilibrium steady state (NESS)* in the sense that the entropy production due to the action of the map over the state is strictly positive. We call them *maps with NESS*. We define *maps with equilibrium* as maps such that the entropy production associated to the action of the map on the invariant state vanishes. From the point of view of thermodynamics, maps with equilibrium have the interesting property that the thermodynamic quantities depend only on system properties even in the strong coupling regime. These maps generalize thermal maps [26] and they are related to the existence of conserved quantities. We also obtain simplifications on the stochastic fluctuations of the thermodynamic quantities.

In a particular limit it is possible to obtain a Lindblad master equation from a repeated interaction scheme or concatenation of CPTP maps. We connect the principle of quantum detailed balance in these master equations to the equilibrium property of the CPTP maps. It has been recently proposed [27] a unifying thermodynamic framework based on repeated interactions to treat systems which cannot be described in the conventional weak coupling regime. We further argue that repeated interactions can be engineered to produce boundary driven Lindblad master equations which might be useful for quantum machines or quantum information processing. This would give a non-trivial consistent thermodynamic framework where the first and second law would work as a guide on the accessibility of states and efficiency of processes, just as the classical first and second laws do for classical heat engines.

This work is organized as follows. In Chapter 1 we write the quantum thermodynamic quantities we will be using, introduce the repeated interaction scheme and apply the special limit in which a Lindblad master equation is obtained. In Chapter 2 we introduce stochastic thermodynamics for CPTP maps, we define CPTP maps with equilibrium and study their main properties and then we prove a fluctuation theorem for the work and entropy production for CPTP maps with and without equilibrium. We also apply our results to a single spin in a thermodynamic cycle and a spin 1/2 chain driven by its boundaries. Finally, in Chapter 3 we relate the detailed balance condition for Lindblad master equations with the equilibrium of CPTP maps, and we show with two examples how to start from a Lindblad equation and derive a repeated interaction that generates it. We conclude afterwards.

Chapter 1

Ensemble thermodynamics

1.1 Thermodynamic quantities

In the thermodynamics of quantum systems it is necessary to define properly heat, work and entropy production, if one wants to have useful quantum thermodynamics laws as in the classical regime. These are fundamental to be able to talk about equilibrium, irreversibility and efficiency. Here we present systematic definitions based on ideas developed in [18]. We remark that there are other valid and consistent definitions which might be more suitable for other contexts [28].

Consider a system initially prepared at time $t = 0$ in an arbitrary state $\rho_S(0)$ and possibly many baths prepared in the canonical thermal state (Gibbsian state) $\rho_r(0) = \omega_{\beta_r}(H_r) \equiv e^{-\beta_r H_r} / Z_r$. Here β_r , H_r and $Z_r = \text{Tr} e^{-\beta_r H_r}$ are the inverse temperature, Hamiltonian and canonical partition function of the bath r , respectively. *We assume that the system and baths are initially uncorrelated.* This assumption is strictly necessary for the positivity of the entropy production definition we give below, i.e., for a consistent second law. The initial total density matrix is

$$\rho(0) = \rho_S(0) \otimes \rho_B(0) = \rho_S(0) \bigotimes_r \rho_r(0). \quad (1.1)$$

ρ denotes the total density matrix of the full system, i.e., the system we are interested in plus all the baths, and $\rho_B(0) = \bigotimes_r \rho_r(0)$ is the density matrix of all the baths. The unitary dynamics of the full system is generated by the total Hamiltonian

$$H(t) = H_S(t) + \sum_r H_r + V(t), \quad (1.2)$$

and can be written as

$$\partial_t \rho(t) = -i[H(t), \rho(t)] \quad (\hbar = 1 \text{ throughout the text}), \quad (1.3)$$

where $H_S(t)$ is the possibly time dependent system Hamiltonian and $V(t)$ is the coupling between the system and the baths. The time dependence of these Hamiltonians indicates

the presence of an external driving. Defining the time ordered unitary operator $U_t = \mathcal{T}_+ \exp(-i \int_0^t ds H(s))$, the total density matrix at time t is

$$\rho(t) = U_t \rho(0) U_t^\dagger. \quad (1.4)$$

This density matrix is generally not a product state like $\rho(0)$. This means that if we partially trace the total density matrix to obtain the reduced density matrix of the system, $\rho_S(t) = \text{Tr}_B[\rho(t)]$, and of the bath, $\rho_B(t) = \text{Tr}_S[\rho(t)]$, we have that $\rho(t) \neq \rho_S(t) \otimes \rho_B(t)$.

At a time t the energy of the total system is given by $E(t) = \text{Tr}[H(t)\rho(t)]$. Derivating with respect to time and noting that $\text{Tr}[H(t)\dot{\rho}(t)] = 0$ because of Eq.(1.3), we obtain $\dot{E} = \text{Tr}[\dot{H}(t)\rho(t)]$. This can be identified as the work (power) due to the fact that it can only be non-zero if there is an external driving in the total Hamiltonian. We thus write $\dot{E}(t) = \dot{W}(t)$, which is the first law of thermodynamics for a isolated system. Integrating in time we have

$$W(t) = \langle H(t) \rangle_t - \langle H(0) \rangle_0 = \int_0^t ds \frac{d}{ds} \text{Tr}[H(s)\rho(s)] = \int_0^t ds (\dot{H}_S(s) + \dot{V}(s))\rho(s), \quad (1.5)$$

where $\langle \bullet \rangle_t \equiv \text{Tr}[\rho(t) \bullet]$.

To construct a definition of entropy production we use the von Neumann entropy which for the full system is given at time t by

$$S(t) \equiv -\text{Tr} \rho(t) \ln \rho(t), \quad (1.6)$$

and for the system ($X = S$) or baths ($X = B$) is

$$S_X(t) \equiv -\text{Tr}_X \rho_X(t) \ln \rho_X. \quad (1.7)$$

The total von Neumann entropy does not change when the evolution is unitary, thus we have $S(t) = S(0)$, which reads

$$\begin{aligned} -\text{Tr} \rho(t) \ln \rho(t) &= -\text{Tr} \rho(0) \ln \rho(0) = -\text{Tr}_S \rho_S(0) \ln \rho_S(0) - \text{Tr}_B \rho_B(0) \ln \rho_B(0) \\ &= -\text{Tr}_S \rho_S(0) \ln \rho_S(0) - \sum_r \text{Tr}_r \rho_r(0) \ln \rho_r(0), \end{aligned} \quad (1.8)$$

where Tr_r denotes the partial trace over the Hilbert space of the bath r . Using this we can write the entropy change of the system, $\Delta S_S(t) = S_S(t) - S_S(0)$, in the following way:

$$\begin{aligned} \Delta S_S(t) &= -\text{Tr}_S \rho_S(t) \ln \rho_S(t) + \text{Tr}_S \rho_S(0) \ln \rho_S(0) \\ &= \text{Tr} \rho(t) \ln \rho(t) - \text{Tr}_S \rho_S(t) \ln \rho_S(t) - \sum_r \text{Tr}_r \rho_r(0) \ln \rho_r(0) \\ &= \text{Tr} \rho(t) \ln \rho(t) - \text{Tr} \rho(t) [\ln \rho_S(t) + \sum_r \ln \rho_r(0)] + \sum_r \text{Tr}_r [(\rho_r(t) - \rho_r(0)) \ln \rho_r(0)] \\ &= \text{Tr} \rho(t) \left[\ln \rho(t) - \ln \left(\rho_S(t) \otimes_r \rho_r(0) \right) \right] + \sum_r \text{Tr}_r [(\rho_r(t) - \rho_r(0)) \ln \rho_r(0)], \end{aligned} \quad (1.9)$$

where $\rho_r(t)$ is the density matrix of the bath r at time t which is the partially traced $\rho(t)$ over all degrees of freedom except those of the bath r . Note that we have added and subtracted the same term in the third line, $\text{Tr}[\rho(t) \sum_r \ln \rho_r(0)] = \sum_r \text{Tr}_r \rho_r(t) \ln \rho_r(0)$. The first term in the last line is the Kullback-Leibler distance or *relative entropy*, $D[a||b] \equiv \text{Tr} a \ln a - \text{Tr} a \ln b \geq 0$, which is zero only when $a = b$. The second term, using the particular form of $\rho_r(0)$, can be rewritten as the inverse temperatures times the heats entering the system

$$\sum_r \beta_r Q_r = \sum_r \beta_r (\langle H_r \rangle_0 - \langle H_r \rangle_t). \quad (1.10)$$

Note that the heats are minus the energy changes of the baths.

The entropy change of the system is separated into two contributions, $\Delta S_S(t) = \Delta_i S(t) + \Delta_e S(t)$, the entropy production

$$\Delta_i S(t) = D[\rho(t) || \rho_S(t) \bigotimes_r \rho_r(0)], \quad (1.11)$$

and the entropy flow entering the system in the form of heat,

$$\Delta_e S(t) = \sum_r \beta_r Q_r(t). \quad (1.12)$$

Now we should unambiguously say that we consider the baths to be useless after the interaction with the system has ended and that they eventually thermalize with the environment (ideal infinite bath). This is clearer if we rewrite the entropy production, Eq.(1.11), as

$$\Delta_i S(t) = D[\rho(t) || \rho_S(t) \bigotimes_r \rho_r(t)] + \sum_r D[\rho_r(t) || \omega_{\beta_r}(H_r)]. \quad (1.13)$$

The first term can be interpreted as the entropy increase due to the correlation built up between the system and the baths, and the second as the dissipation that occurs in the relaxation process $\rho_r(t) \rightarrow \omega_{\beta_r}(H_r)$ [29] (or in connection with quantum information, as the lack of information about the state of the bath after the interaction [27]).

The splitting of the entropy change of the system in two contributions and the non-negativity of the entropy production, Eq.(1.11), corresponds to the second law of thermodynamics for an open system. Now, for this open system the work is still given by Eq.(1.5). In order to be consistent with the heats definitions, Eq.(1.10), we must define the internal energy as the energy of the system and the coupling, i.e., as $U(t) = \langle H_S(t) + V(t) \rangle_t$. The change $\Delta U(t) = U(t) - U(0)$ is

$$\Delta U(t) = \langle H_S(t) + V(t) \rangle_t - \langle H_S(0) + V(0) \rangle_0. \quad (1.14)$$

We thus have the first law, $\Delta U(t) = W(t) + Q(t)$.

We remark that the definition of entropy production, Eq.(1.11), and its positivity holds for any bath size.

In the following we use time independent system Hamiltonians to emphasize that work can be done by just manipulating the coupling $V(t)$, driving the system out of equilibrium. At the moment this might seem obvious, but later on we will obtain Lindblad equations widely used in the literature [30, 31, 32, 16, 33] in which this active driving origin is hidden.

1.2 Repeated interaction

We now introduce the *repeated interaction scheme* where a system of interest interacts sequentially with other systems.

Consider a finite system with time independent Hamiltonian H_S and possibly many baths, each one consisting of a set of identical non-interacting finite systems with Hamiltonians H_r^n . This means that the bath r has Hamiltonian $H_r = \bigoplus_n H_r^n$. We shall call H_r^n the n th copy of the r th bath. The system and baths are initially uncorrelated, as in Eq.(1.1), where $\rho_r(0) = \bigotimes_n \rho_r^n(0) = \bigotimes_n \omega_{\beta_r}(H_r^n)$. The interaction between the system and the baths is divided into N steps of time τ from $t = 0$ to $t = T = N\tau$. In the n th time step the system-bath coupling is a time-independent $V^n = \sum_r V_r^n$, this means that there is a different unitary evolution operator U_n for each step. At $t = 0^+$ the first copy of each bath starts to interact with the system until time $t = \tau$, when the total density matrix is $\rho(\tau) = U_1(\rho_S(0) \otimes \rho_1)U_1^\dagger \otimes \rho_2 \otimes \rho_3 \otimes \dots$, where $\rho_n = \bigotimes_r \rho_r^n(0)$ contains the n th copy of every bath. From time $t = \tau^+$ to $t = 2\tau$ the second copy of each bath interacts with the system and the total density matrix becomes $\rho(2\tau) = \mathcal{U}_2 \left(U_1(\rho_S(0) \otimes \rho_1)U_1^\dagger \otimes \rho_2 \right) \mathcal{U}_2^\dagger \otimes \rho_3 \dots$. Tracing out the baths a recurrence for the system density matrix is found:

$$\rho_S(n\tau) = \text{Tr}_B[U_n \rho_S((n-1)\tau) \otimes \rho_n U_n^\dagger]. \quad (1.15)$$

The unitary operators are $U_n = e^{-i\tau(H_S + \sum_r H_r^n + V_r^n)}$ and $\mathcal{U}_n = U_n \prod_{m=1}^{n-1} e^{-i\tau \sum_r H_r^m}$ (hereinafter $\hbar = 1$). Note that the time dependence of the coupling, $V(t) = V^n$ if $t \in ((n-1)\tau, n\tau]$, corresponds to turning off the interaction with a copy and turning on the interaction with the next copy. In Fig. 1.1 a picture of the repeated interaction scheme is shown.

During the n th time interval, according to the definitions in the previous section, heat and work are

$$\sum_r \Delta Q_r^{n\tau} = \text{Tr}_r[H_r^n(\rho_n - \rho'_n)], \quad \sum_r \Delta W_r^{n\tau} = -\text{Tr}[V_r^n U_n \rho_S((n-1)\tau) \otimes \rho_n U_n^\dagger], \quad (1.16)$$

where $\rho'_n = \text{Tr}_S[U_n \rho_S((n-1)\tau) \otimes \rho_n U_n^\dagger]$ corresponds to the n th copies of the baths after the interaction. We have written Δ to emphasize that these are the heat and work in only one interval. The heat expression is obtained straightforwardly. For the work expression, note that H_S does not depend on time and $V(t)$ only changes at the end of the interval. In Eq.(1.5) one integrates in the small interval $(n\tau - \epsilon, n\tau + \epsilon)$, which is when V changes, and takes the limit $\epsilon \rightarrow 0$ afterwards. Then, the expression $\text{Tr}[(V^{n+1} - V^n)\rho]$ is simplified assuming that $\text{Tr}_r[V_r^n \omega_{\beta_r}(H_r^n)] = 0$ (this is a common assumption and it is always possible to redefine the Hamiltonians of a given total system so that it is satisfied). Heat and work in the whole process is obtained summing over every interval the previous expressions.

According to Eqs.(1.11) or (1.13), the entropy production during the n th time interval is

$$\Delta_i S^{n\tau} = D[U_n \rho_S((n-1)\tau) \otimes \rho_n U_n^\dagger || \rho_S(n\tau) \otimes \rho'_n] + D[\rho'_n || \rho_n]. \quad (1.17)$$

(Again here Δ indicates this is the entropy production in just one interval.)

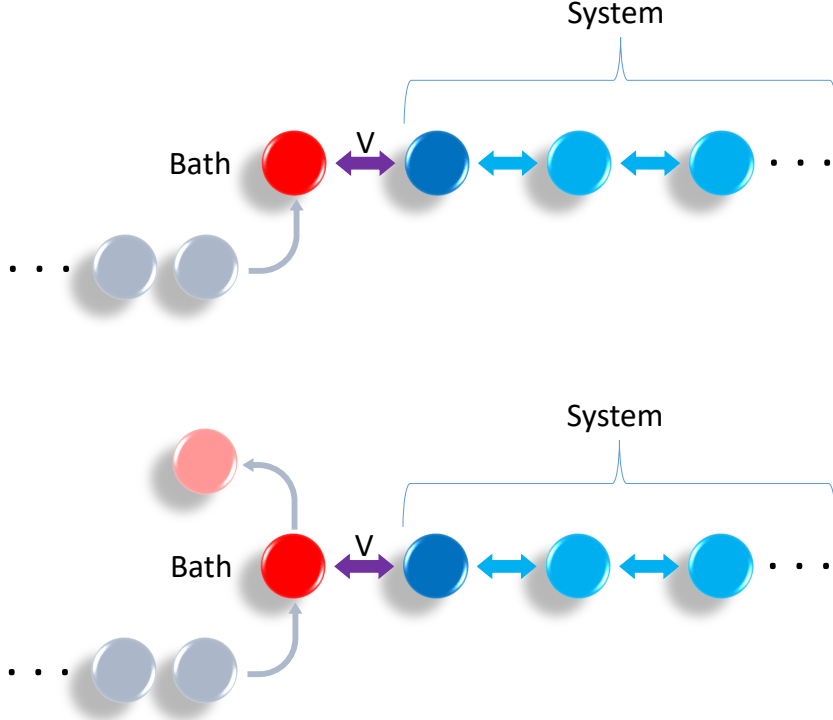


Figure 1.1: Depiction of the first two interactions between a spin chain system (considered in our examples in Sec. 2.6) and the copies of the bath.

1.2.1 Continuous limit

If the couplings between the system and the baths scale as $V^n = v^n/\sqrt{\tau}$, in the limit $\tau \rightarrow 0$ and $n \rightarrow \infty$ such that $t = n\tau$, one can obtain a continuous equation for the evolution of the system density matrix [34, 35, 16]. Expanding $\Delta\rho_S \equiv \rho_S((n+1)\tau) - \rho_S(n\tau)$ to first order in τ one obtains

$$\Delta\rho_S = -i\tau[H_S, \rho_S] + \tau \text{Tr}_B[v^n \rho_S(n\tau) \otimes \rho_B v^n] - \frac{1}{2}\tau \text{Tr}_B\{(v^n)^2, \rho_S \otimes \rho_B\} + \mathcal{O}(\tau^{3/2}), \quad (1.18)$$

where $\rho_B = \bigotimes_r \rho_r(0)$, and $[\bullet, \bullet]$ and $\{\bullet, \bullet\}$ denotes the commutator and anticommutator, respectively. It was used that $\text{Tr}_B[H_B, \rho_B] = 0$ and $\text{Tr}_B[v^n \rho_B] = 0$. Dividing by τ , taking the limits and splitting the coupling one obtains

$$\dot{\rho}_S = -i[H_S, \rho_S] + \sum_r \mathcal{D}_r(\rho_S), \quad (1.19)$$

where the dissipators are $\mathcal{D}_r(\rho_S) = \text{Tr}_r[v_r \rho_S \otimes \omega_{\beta_r} v_r] - \frac{1}{2} \text{Tr}_r\{v_r^2, \rho_S \otimes \omega_{\beta_r}\}$. For the heat of the r th bath, expanding the unitary operator up to order τ and taking the limits we obtain the heat flow

$$\dot{Q}_r(t) = \lim_{n \rightarrow \infty} \lim_{\tau \rightarrow 0} \frac{\Delta Q_r^{n\tau}}{\tau} = -\text{Tr} \left[\left(v_r H_r v_r - \frac{1}{2} \{v_r^2, H_r\} \right) \rho_S(t) \otimes \omega_{\beta_r} \right] \quad (1.20)$$

Note that V_r^n appears in the work in Eq.(1.16), thus to obtain the work in the continuous limit we need to expand the unitary operator up to order $\tau^{3/2}$. We get for each bath a power

$$\dot{W}_r(t) = \lim_{n \rightarrow \infty} \lim_{t \rightarrow 0} \frac{\Delta W_r^{n\tau}}{\tau} = \text{Tr} \left[\left(v_r(H_S + H_r)v_r - \frac{1}{2}\{v_r^2, H_S + H_r\} \right) \rho_S(t) \otimes \omega_{\beta_r} \right]. \quad (1.21)$$

Note that using the permutation invariance of the trace we get that the first law is satisfied, $\sum_r (\dot{Q}_r + \dot{W}_r) = \text{Tr}[H_S \dot{\rho}_S]$.

The dissipator of Eq.(1.19) can be expanded in the bath energy basis, $\{|\varepsilon_i\rangle\}$ and one obtains

$$\dot{\rho}_S = -i[H_S, \rho_S] + \sum_{rij} \gamma_{ij}^r (L_{ij} \rho_S L_{ij}^\dagger - \frac{1}{2}\{L_{ij}^\dagger L_{ij}, \rho_S\}), \quad (1.22)$$

where $\gamma_{ij} = e^{-\beta\varepsilon_i}/Z_B$ and $L_{ij}^r = \langle \varepsilon_j | v_r | \varepsilon_i \rangle$. This master equation is of Lindblad form [15].

1.2.2 Lindblad limit for the XX and XY spin chains

Later on we will apply our results to a few examples, mainly the XX and XY spin 1/2 chains. For this reason, we now develop the Lindblad form of the continuous limit of the previous subsection for these particular systems and point out some of the main results in [16] regarding the thermodynamics of these systems.

Consider a system Hamiltonian

$$H_{XY} = \frac{\hbar}{2} \sum_{i=1}^N \sigma_i^z - \sum_{i=1}^{N-1} (J_i^x \sigma_i^x \sigma_{i+1}^x + J_i^y \sigma_i^y \sigma_{i+1}^y). \quad (1.23)$$

where $\sigma_i^{x,y,z}$ are the Pauli matrices of the site i . This is the Hamiltonian of the XY one-dimensional spin 1/2 chain of N spins. For the XX spin chain Hamiltonian, H_{XX} , the coupling in both directions are equal, $J_i^x = J_i^y$.

For simplicity and because it is sufficiently interesting for the analysis we want to do, we will choose to connect only one bath (with inverse temperature β_L) to the system at its boundary, at the left hand side of the spin chain. Each bath copy is a 1/2 spin with Hamiltonian $H_L = \frac{\hbar L}{2} \sigma_L^z$, where L indicates that the bath is coupled to the system by the left, next to the $n = 1$ spin of the chain. The coupling between a copy of the bath and the system is

$$V = J(\sigma_L^x \sigma_1^x + \sigma_L^y \sigma_1^y). \quad (1.24)$$

Note that we have dropped the superscript n in the coupling, since no confusion will arise: the coupling is the same for each bath copy.

Scaling the system-bath coupling coefficient $J = \sqrt{\lambda/\tau}$ and replacing everything in Eq.(1.19) one obtains a dissipator

$$\mathcal{D}(\rho_S) = \sum_{k=\pm} \gamma_k \left(L_k \rho_S L_k^\dagger - \frac{1}{2}\{L_k^\dagger L_k, \rho_S\} \right), \quad \gamma_{\pm} = \sqrt{2\lambda(1 \mp \tanh(\beta_L \hbar L/2))} \quad (1.25)$$

with Lindblad operators $L_{\pm} = \sigma_1^{\pm}$, where $\sigma_1^{\pm} = (\sigma_1^x \pm i\sigma_1^y)/2$. Note that this dissipater does not depend in the system Hamiltonian, thus is the same for the XX and XY systems. Note also that it corresponds to a boundary driven Lindblad equation in which the Lindblad operators are not eigenoperators of the complete system Hamiltonian, but only of a part of the system Hamiltonian. We will come back to this point in Section 3 where conserved quantities in the Lindblad limit are discussed.

In [16] there are two important results regarding the XX and XY systems coupled to one bath that we will need:

1. If $h_L = h$, the XX spin chain reaches *equilibrium*, i.e., heat flow, power and entropy production rate vanish. The equilibrium state is not Gibbsian ($e^{-\beta H_S}/Z_S$), but it is a state given by $e^{-\beta H_0}/Z_0$ with $H_0 = h/2 \sum_i \sigma_i^z$ a conserved quantity of the system, $[H_S, H_0] = 0$, and Z_0 the normalization.
2. The XY spin chain coupled to one bath reaches a *non-equilibrium steady state* (NESS), i.e., entropy production rate is positive, and a heat flux is dissipated due to the driving power, $\dot{W} = -\dot{Q} > 0$.

It is important to mention that these results are not only valid in the continuous limit, but also in the time-discrete repeated interaction scheme, Eqs.(1.16, 1.17).

The formalism of repeated interaction in the Lindblad limit was used to establish a consistent relation between boundary driven Lindblad equations and thermodynamics, a relation which has been questioned before.

Chapter 2

Stochastic thermodynamics in the quantum regime

2.1 CPTP maps

The formalism of quantum operations is a very important tool in the context of quantum information processing (see e.g. [17]), since it can describe changes in the state of a open quantum system without explicitly paying attention to the time that is needed nor to all the information of the environment. In the first respect, this is very different from the usual description of open quantum systems, which are master equations as the Lindblad form discussed above.

Completely positive trace preserving (CPTP) quantum maps are an important class of quantum operations. They can be used to describe the dynamics of thermal relaxation, decoherence and measurement, among others. Any CPTP quantum map $\rho_S \rightarrow \rho'_S \equiv \mathcal{E}(\rho_S)$ allows the following *Kraus representation* (or *operator-sum representation*)

$$\mathcal{E}(\rho_S) = \sum_k M_k \rho_S M_k^\dagger, \quad (2.1)$$

where linear operators $\{M_k\}$ are called *Kraus operators* (or *operation elements*) and satisfy the *completeness relation* $\sum_k M_k^\dagger M_k = \mathbb{1}$, which is necessary to ensure the trace preserving property. Note that the choice of Kraus operators for a given map is not unique, since any unitary transformation of $\{M_k\}$ fulfils the same requirements. However, as we will see next, one can gain important insight into the dynamics with an appropriate choice of Kraus operators.

2.2 Quantum trajectories

Any system that couples to an environment and the composite system has unitary dynamics for a time interval, for instance Eq.(1.15), has an evolution that is a CPTP map:

$$\begin{aligned}
\rho'_S &= \mathcal{E}(\rho_S) = \text{Tr}_B[U \rho_S \otimes \rho_B U^\dagger] \\
&= \sum_i p_i \text{Tr}_B[U \rho_S \otimes |i\rangle \langle i| U^\dagger] \\
&= \sum_{ij} p_i \langle j| U |i\rangle \rho_S \langle i| U^\dagger |j\rangle \\
&= \sum_{ij} M_{ij} \rho_S M_{ij}^\dagger,
\end{aligned} \tag{2.2}$$

where

$$M_{ij} = \sqrt{p_i} \langle j| U |i\rangle \tag{2.3}$$

is an operator in the system space with $\{|i\rangle\}$ and $\{p_i\}$ the states and probabilities that diagonalize $\rho_B = \sum_i p_i |i\rangle \langle i|$. If $\{ij\}$ is taken to be just one label, this is a CPTP map like the one in Eq.(2.1) and fulfils the completeness relation.

We can split the map as $\mathcal{E}(\cdot) = \sum_k \mathcal{E}_k(\cdot)$, where $\mathcal{E}_k(\cdot) = M_k \cdot M_k^\dagger$. During the evolution one of the operations \mathcal{E}_k occurs with probability $p_k = \text{Tr}[\mathcal{E}_k(\rho_S)]$. If somehow one is able to register that the k th operation has occurred, the final state of the system would be $\rho'_k = \mathcal{E}_k(\rho_S)/p_k$, whereas if one is not able to record it, the final state would be $\rho'_S = \sum_k p_k \rho'_k = \mathcal{E}(\rho_S)$. This suggests the interpretation that one measures selectively or non-selectively the occurrence of the element M_k .

Suppose an arbitrary initial density matrix of the system is prepared measuring non-selectively a non-degenerate operator A in the system's Hilbert space. We shall denote ρ_S^{ini} the arbitrary initial density matrix and $\rho_S = \sum_n p_i(n) |a_n\rangle \langle a_n|$ the density matrix after the non-selective measurement of A , where $\{|a_n\rangle\}$ are the eigenstates of A . Then, the system evolves through the map \mathcal{E} . After the evolution we perform a non-selective measurement of a non-degenerate operator B in the Hilbert space of the system, leaving the state ρ'_S in $\bar{\rho}'_S = \sum_b p_f(m) |b_m\rangle \langle b_m|$, where $\{|b_m\rangle\}$ are the eigenstates of B . A trajectory is defined as the sequence of possible values a_n , k and b_m that would be obtained if the measurements were done selectively, and is denoted $\gamma = \{n, k, m\}$. Its probability is given by

$$p(\gamma) = p_i(n) \langle b_m| \mathcal{E}_k(|a_n\rangle \langle a_n|) |b_m\rangle = p_i(n) |\langle b_m| M_k |a_n\rangle|^2, \tag{2.4}$$

this is, the probability of measuring b_m given that the operation k has occurred and that a_n was initially measured. Note that the probabilities sum one, in fact $\sum_\gamma p(\gamma) = \text{Tr}[\mathcal{E}(\rho_S)] = 1$.

As we mentioned before, an appropriate choice of Kraus operators can give us an interesting insight. If $M_{k=ij} = \sqrt{p_i} \langle j| U |i\rangle$, the register of k is the register of a jump $|i\rangle \rightarrow |j\rangle$ in the bath. Thus, to observe a particular trajectory one can use a *two-point measurement scheme*, i.e., one measures the system and baths before and after the interaction, obtaining values $\{n, k, m\} = \{n, i, j, m\}$. In the case of our repeated interaction model, the Hamiltonian of

the bath is a two-level system thus one could easily perform a two-point measurement of the energy and determine precisely a transition between states. However, if one is interested in more general models where baths have many degrees of freedom, it is unrealistic to assume that energy transitions could be directly measured in the bath. An alternative then would be to let a quantum probe interact with the bath. Measuring the probe one would be able to identify energy changes in the bath, which is very useful for the stochastic thermodynamics.

2.3 Stochastic thermodynamics

For the definition of trajectory made above, we will now study the thermodynamic quantities associated with it. Suppose the operators A and B of the previous section are the Hamiltonian of the system, H_S . We assume, as in Section 1.2, that the system and bath Hamiltonians are time independent. If ρ_B is Gibbsian (canonical), then the states $\{|i\rangle\}$ are the energy eigenstates of the bath Hamiltonian H_B with eigenvalues $\{\varepsilon_i\}$. With this in mind, in a particular trajectory $\gamma = \{n, i, j, m\}$ a stochastic work

$$w_\gamma = \Delta\epsilon - q_\gamma \quad (2.5)$$

is done on the system, where

$$\Delta\epsilon_\gamma = \epsilon_m - \epsilon_n \quad \text{and} \quad q_\gamma = \varepsilon_i - \varepsilon_j \quad (2.6)$$

are the stochastic energy change of the system and the stochastic heat entering the system (which is minus the stochastic energy change of the bath), respectively. This is the first law of stochastic thermodynamics [36, 37]. Averaging over the trajectories one obtains

$$\Delta E \equiv \langle \Delta\epsilon_\gamma \rangle_\gamma = \sum_\gamma \Delta\epsilon_\gamma p(\gamma) = \text{Tr}[H_S(\rho'_S - \rho_S)] = \text{Tr}[H_S(\rho'_S - \rho_S^{\text{ini}})], \quad (2.7)$$

$$Q \equiv \langle q_\gamma \rangle_\gamma = \sum_\gamma q_\gamma p(\gamma) = \text{Tr}[H_B(\rho_B - \rho'_B)], \quad (2.8)$$

$$W \equiv \langle w_\gamma \rangle_\gamma = \sum_\gamma w_\gamma p(\gamma) = \text{Tr}[(H_S + H_B)(\rho' - \rho)] = \text{Tr}[(H_S + H_B)(\rho' - \rho^{\text{ini}})]. \quad (2.9)$$

(Note that in the last step of the energy change and work we have used that ρ_S and ρ are diagonal in the basis of H_S and $H_S + H_B$, respectively, thus $\text{Tr}[H_S\rho_S] = \text{Tr}[H_S\rho_S^{\text{ini}}]$ and $\text{Tr}[(H_S+H_B)\rho] = \text{Tr}[(H_S+H_B)\rho^{\text{ini}}]$.) These equations satisfy the first law of thermodynamics. We remark that we have implicitly considered that the system and bath Hamiltonians, H_S and H_B , are time-independent and thus their eigenvalues and eigenstates are the same in the first and second measurements. In the same spirit of Section 1.2 work can on average be done on the system by applying a map. Turning on and off a system-bath coupling is also an application of consecutive maps. We will discuss these in Section 2.5.

If the unitary dynamics of Eq.(2.2) are generated by a total time-independent Hamiltonian $H = H_S + H_B + V$, where V is the system-bath coupling as usual, we have that our averaged stochastic work is equal to $-\text{Tr}[V(\rho' - \rho)]$, since $\text{Tr}[H(\rho' - \rho)] = 0$ due to the fact that $[H, U] = 0$. If we make the already mentioned assumption $\text{Tr}_B[V\rho_B] = 0$, we get $W =$

$-\text{Tr}[V\rho']$. This is just the ensemble average Eq.(1.16) in the repeated interaction scheme in the case of just one iteration. The average of the stochastic energy change and heat are clearly the same as their ensemble average counterparts.

Information about stochastic entropy change can also be obtained with the measurements choosing different operators A and B . Although it is absolutely non-trivial from an experimental point of view, measuring the system density matrix at the beginning and at the end of the process, $A = \rho_S$ and $B = \rho'_S$, one can construct the stochastic entropy change of the system, $\Delta s_\gamma = -\ln p_f(m) + \ln p_i(n)$. It is in principle possible to completely reconstruct a density matrix through quantum state tomography, but the number of measurements needed for this procedure scales exponentially with the system size. Anyhow, with Δs_γ and the heat q_γ , which is known due to the measurements on the bath, one obtains the stochastic entropy production

$$\Delta_i s_\gamma = \Delta s_\gamma - \beta q_\gamma. \quad (2.10)$$

Averaging over the trajectories one obtains

$$\Delta S \equiv \langle \Delta s_\gamma \rangle_\gamma = \sum_\gamma \Delta s_\gamma p(\gamma) = -\text{Tr}[\rho'_S \ln \rho'_S] + \text{Tr}[\rho_S \ln \rho_S] \quad (2.11)$$

$$\Delta_i S \equiv \langle \Delta_i s_\gamma \rangle_\gamma = D[\rho' || \rho'_S \otimes \rho_B]. \quad (2.12)$$

In the second expression we have used that $\ln \rho_B = -\beta H_B - \ln Z_B$ and that $\text{Tr}[\rho' \ln \rho'] = \text{Tr}[\rho \ln \rho] = \text{Tr}[\rho_S \ln \rho_S] + \text{Tr}[\rho_B \ln \rho_B]$ (the unitary dynamics do not modify the total von Neumann entropy). Note that this averaged stochastic entropy production is the same as the ensemble entropy production of Eq.(1.11).

We remark that for the evaluation of these thermodynamic quantities, in particular for the work, Eq.(2.9), and entropy production, Eq.(2.12), we need to know the full state ρ' . In contrast, in the weak coupling limit where $V(t)$ can be neglected in comparison to H_S and H_B the thermodynamic quantities depend only on the states ρ'_S and ρ_S of the system of interest [15]. We will show below, that this simplification can occur for the strongly coupled systems defined below.

2.3.1 Maps with thermodynamic equilibrium and conserved quantities

Let us assume that the CPTP map \mathcal{E} of Eq.(2.2) has an invariant state $\pi = \mathcal{E}(\pi)$ that is a stationary state, i.e., $\lim_{N \rightarrow \infty} \mathcal{E}^N(\rho_S) = \pi \forall \rho_S$. According to Eq.(2.2) an *invariant state* satisfy $\pi = \text{Tr}_B[U(\pi \otimes \rho_B)U^\dagger]$, thus from Eqs.(2.7) and (2.11) we see that it has no energy nor entropy change, $\Delta E = \Delta S = 0$. We shall now distinguish two kinds of invariant states. If the action of the map \mathcal{E} over π produces entropy, $\Delta_i S > 0$, we say that the invariant state is a *non-equilibrium stationary state* (NESS). In that case we get a dissipated heat $Q = -\beta^{-1} \Delta_i S < 0$ sustained by a work $W = \beta^{-1} \Delta_i S > 0$ done over the system by an external agent that implements the map on the system. If instead the action of the map does not produce entropy, $\Delta_i S = 0$, we call the invariant state π an *equilibrium state*. According to Eq.(2.12), an equilibrium state is only possible if $\pi \otimes \omega_\beta(H_B) = U(\pi \otimes \omega_\beta(H_B))U^\dagger$, thus from Eqs.(2.8) and (2.9) we see that it has no average heat or work.

The equilibrium state is associated with conserved quantities. To see this suppose there is a system operator H_0 in the system Hilbert space \mathcal{H}_S with the property $[U, H_0 + H_B] = 0$. We recall that the initial state of the bath is Gibbsian, $\rho_B = \omega_\beta(H_B) = e^{-\beta H_B}/Z_B$, thus if $\pi = \omega_\beta(H_0)$ then it is a equilibrium state since $U(\omega_\beta(H_0) \otimes \omega_\beta(H_B))U^\dagger = \omega_\beta(H_0) \otimes \omega_\beta(H_B)$. If H_0 is a part of the system Hamiltonian, $H_S = H_0 + H_I$, like the case of the XX spin chain we study in the applications at the end of this chapter, the equilibrium condition means that the energy change between H_0 and the bath is conserved.

It follows from $[U, H_0 + H_B] = 0$ that

$$\mathrm{Tr}_S[(\rho'_S - \rho_S) \ln \omega_\beta(H_0)] = \mathrm{Tr}_B[(\rho_B - \rho'_B) \ln \omega_\beta(H_B)]. \quad (2.13)$$

This is obtained noting that $\mathrm{Tr}_S[(\rho'_S - \rho_S) \ln \omega_\beta(H_0)] + \mathrm{Tr}_B[(\rho'_B - \rho_B) \ln \omega_\beta(H_B)] = \mathrm{Tr}[(\rho' - \rho) \ln(\omega_\beta(H_0) \otimes \omega_\beta(H_B))] = 0$ because of $[U, \ln(\omega_\beta(H_0) \otimes \omega_\beta(H_B))] = 0$. This is true for any initial states ρ_S and ρ_B . In particular, for $\rho_B = \omega_\beta(H_B)$, the thermodynamics quantities, Eqs.(2.8), (2.9) and (2.12) can be rewritten in the following way:

$$Q = \mathrm{Tr}_B[H_0(\rho'_S - \rho_S)], \quad (2.14)$$

$$W = \mathrm{Tr}_S[(H_S - H_0)(\rho'_S - \rho_S)], \quad (2.15)$$

$$\Delta_i S = D(\rho_S || \omega_\beta(H_0)) - D(\rho'_S || \omega_\beta(H_0)). \quad (2.16)$$

These expressions are exact and are determined by the system states ρ'_S and ρ_S only, even in the strong coupling regime (since no assumption on the coupling has been made).

2.3.2 Stochastic thermodynamics of thermal maps

If $H_0 = H_S$ the map is called *thermal* [38, 39, 40, 26]. In this case the equilibrium state is the Gibbs canonical thermal state $\omega_\beta(H_S) = e^{-\beta H_S}/Z_S$. Thermal maps are supposed to describe the passive coupling between a system and bath because it requires no external agent. This is not only evidenced in that the average work vanishes, but also in that there are no work fluctuations. To see this note that if a trajectory is possible ($p(\gamma) \sim |\langle \epsilon_m, \epsilon_j | U | \epsilon_n, \epsilon_i \rangle|^2 \neq 0$), then due to $[U, H_S + H_B] = 0$ the energy must be conserved, $\epsilon_m + \epsilon_j = \epsilon_n + \epsilon_i$. Therefore, for a thermal map, Eq.(2.5) gives $w_\gamma = 0$ for any trajectory γ with $p(\gamma) \neq 0$ and for any initial state ρ_S^{ini} .

If a thermal map brings the system to the equilibrium, the entropy production, Eq.(2.16), reduces to just the first term, $\Delta_i S = D(\rho_S || \omega_\beta(H_S))$. This is a well known expression [29] and is interpreted as the dissipation occurring in the relaxation process $\rho_S \rightarrow \omega_\beta(H_S)$.

Suppose now that the system starts in equilibrium, $\rho_S = \rho'_S = \omega_\beta(H_S)$. According to Eq.(2.16), in this case the entropy production vanishes. Also there are no entropy production fluctuations because $\Delta s_\gamma = \beta \Delta e_\gamma$ and according to what have been said about its work fluctuations, we have that $q_\gamma = \Delta e_\gamma$, thus $\Delta_i s_\gamma = 0$ (see Eq.(2.10)) for every possible trajectory, $p(\gamma) \neq 0$.

Note that for thermal maps in the equilibrium state work an entropy production fluctuations can be considered simultaneously since $[H_S, \omega_\beta(H_S)] = 0$, or in words, measuring the energy or the density matrix is the same.

2.3.3 Stochastic thermodynamics of non-thermal maps with equilibrium

If $H_0 \neq H_S$ is a conserved quantity we have called it a map with a (non-thermal) equilibrium state. We will restrict ourselves to this case, where $[H_S, H_0] = 0$. This is the situation we will encounter in the examples we use and we argue that it will often be the case if the system Hamiltonian is constant in time, $H_S(t) = H_S$, and the coupling is a step function, i.e., $V(t) = V$ if $0 < t < \tau$ and $V(t) = 0$ otherwise, as in the examples of the boundary driven XX and XY spin 1/2 chains in the repeated interaction scheme discussed in Section 1.2. In fact, the equilibrium property $[U, H_0 + H_B] = 0$ implies that $[H_S, H_0] = 0$ for most systems, with the exception of some very particular cases in which $[V, H_0 + H_B] = [H_0, H_S] \otimes \mathbb{1}_B$. Anyhow, if $[H_S, H_0] = 0$ the first interesting observation is that, since H_S is assumed non-degenerated (otherwise there would be problems defining a trajectory), the eigenbasis $\{|\epsilon_n\rangle\}$ of H_S is also an eigenbasis of H_0 , i.e., $H_0 |\epsilon_n\rangle = \epsilon_n^0 |\epsilon_n\rangle$. Then, from the equilibrium property, $[U, H_0 + H_B] = 0$, one finds that $\epsilon_m^0 + \epsilon_j = \epsilon_n^0 + \epsilon_i$ if $p(\gamma) \sim |\langle \epsilon_m, \epsilon_j | U | \epsilon_n, \epsilon_i \rangle|^2 \neq 0$. Therefore, we can write Eq.(2.5) as $w_\gamma = \epsilon_m - \epsilon_m^0 - (\epsilon_n - \epsilon_n^0)$ and replace it inside the delta function of the work distribution $p(w) = \sum_\gamma \delta(w - w_\gamma) p_\gamma$, obtaining

$$p(w) = \sum_{n,m} \delta(w - [(\epsilon_m - \epsilon_m^0) - (\epsilon_n - \epsilon_n^0)]) p_i(n) \langle \epsilon_m | \mathcal{E}(|\epsilon_n\rangle \langle \epsilon_n|) | \epsilon_m \rangle. \quad (2.17)$$

It is completely determined by system quantities and the map \mathcal{E} without the need of measuring the bath. The average of the work with this distribution corresponds to Eq.(2.15). Note that since we are considering $[H_S, H_0] = 0$ it is always possible to write $H_S = H_0 + H_I$ with some H_I that commutes with the system Hamiltonian, $[H_S, H_I] = 0$, and shares the same eigenbasis. Thus, we can split the eigenenergy $\epsilon_n = \epsilon_n^0 + \alpha_n$ with α_n the eigenvalue of H_I . The stochastic work is then $w_\gamma = \alpha_m - \alpha_n$ and its average, Eq.(2.15), is $W = \text{Tr}_S[H_I(\rho'_S - \rho_S)]$.

In the same manner as with thermal maps, we can study simultaneously the work and entropy production fluctuations in the equilibrium state of these equilibrium maps because H_S commutes with $\omega_\beta(H_0)$. One analogously finds here that there are no entropy fluctuations, $\Delta_i s_\gamma = 0 \forall \gamma$ with $p(\gamma) \neq 0$, i.e., $p(\Delta_i s) = \sum_\gamma \delta(\Delta_i s - \Delta_i s_\gamma) p(\gamma) = \delta(\Delta_i s)$, but there might be work fluctuations (in general $p(w)$ given by Eq.(2.17) is different from $\delta(w)$) even though the average vanishes, $W = 0$.

2.4 Fluctuation theorems

2.4.1 Fluctuations of entropy production

A central result from stochastic thermodynamics is the detailed fluctuation theorem for the stochastic entropy production $\Delta_i s$. Consider the probability distribution $p(\Delta_i s) = \sum_\gamma \delta(\Delta_i s - \Delta_i s_\gamma) p(\gamma)$ of a given $\Delta_i s$ value obtained according to the $A = \rho_S$ and $B = \rho'_S$ two-point measurement procedure. The detailed fluctuation theorem for the entropy production

is

$$\ln \frac{p(\Delta_i s)}{\tilde{p}(-\Delta_i s)} = \Delta_i s, \quad (2.18)$$

where $\tilde{p}(\Delta_i s)$ refers to the distribution of the entropy production in a reverse process to be specified later. This equality is derived from the time reversal properties of the system. For the type of systems we study it was derived in [22] for driven Hamiltonians. Here we derive it to emphasize that the fluctuation theorem is also valid for systems driven by other mechanisms, for instance, by the coupling to the bath.

The time reversal operator [41] Θ is anti-unitary, i.e., $\Theta i = -i\Theta$, $\Theta^\dagger = \Theta^{-1}$. This operator is defined in the full Hilbert space $\mathcal{H}_S \otimes \mathcal{H}_B$ and is of the form $\Theta_S \otimes \Theta_B$. The unitary evolution U depends on the time dependence of the coupling that at least is switched on and off. This time dependence is referred to as the protocol. If one performs the protocol in the time inverted sequence, i.e., one considers $V(\tau - t)$ the unitary dynamics will be called \tilde{U} . The micro-reversibility principle for non-autonomous systems [42, 43] relates the forward and backward dynamics by $\Theta^\dagger \tilde{U} \Theta = U^\dagger$. Thus if the unitary operator maps $|\phi\rangle$ to $|\phi'\rangle$, i.e., $|\phi'\rangle = U|\phi\rangle$, the time reversed state $\Theta|\phi'\rangle$ is mapped to the time reversed state $\Theta|\phi\rangle$ by the time reversed unitary \tilde{U} . We denote reverse states as $|\tilde{\cdot}\rangle = \Theta|\cdot\rangle$. We remark that the anti-linearity of Θ implies that $\langle \tilde{\cdot} | = \langle \Theta \cdot | \neq \langle \cdot | \Theta^\dagger$.

For the time reversed dynamics consider the initial state $\tilde{\rho}_S = \sum \tilde{p}_f(m) |\tilde{b}_m\rangle \langle \tilde{b}_m|$ which is chosen arbitrarily for the system and thermal for the bath $\tilde{\rho}_B = \sum \frac{e^{-\beta \varepsilon_j}}{Z_B} |\tilde{j}\rangle \langle \tilde{j}|$. Then, for the system the corresponding time reversed map $\tilde{\rho}'_S = \tilde{\mathcal{E}}(\tilde{\rho}_S)$ has the representation $\tilde{\mathcal{E}}(\cdot) = \sum_{ij} \tilde{M}_{ji} \cdot \tilde{M}_{ji}^\dagger$ in terms of reversed Kraus operators

$$\tilde{M}_{ji} = \sqrt{\frac{e^{-\beta \varepsilon_j}}{Z_B}} \langle \tilde{i} | \tilde{U} | \tilde{j} \rangle. \quad (2.19)$$

Micro-reversibility implies that they satisfy (see Appendix A)

$$\tilde{M}_{ji} = \Theta_S \sqrt{e^{\beta(\varepsilon_i - \varepsilon_j)}} M_{ij}^\dagger \Theta_S^\dagger. \quad (2.20)$$

We can now relate the probability $p(\gamma) = |\langle b_m | M_{k=ij} | a_n \rangle|^2 p_i(n)$ for a trajectory $\gamma = \{n, k, m\} = \{n, i, m, j\}$ to the probability $\tilde{p}(\tilde{\gamma}) = |\langle \tilde{a}_n | M_{k=ji} | \tilde{b}_m \rangle|^2 \tilde{p}_f(m)$ of its time reversal $\tilde{\gamma} = \{\tilde{m}, \tilde{k}, \tilde{n}\} = \{\tilde{m}, \tilde{j}, \tilde{n}, \tilde{i}\}$. From Eq.(2.20) we have $\tilde{p}(\tilde{\gamma}) = e^{\beta(\varepsilon_i - \varepsilon_j)} |\langle a_n | M_{k=ij}^\dagger | b_m \rangle|^2 \tilde{p}_f(m)$ and therefore

$$\frac{p(\gamma)}{\tilde{p}(\tilde{\gamma})} = e^{-\beta(\varepsilon_i - \varepsilon_j)} \frac{p_i(n)}{\tilde{p}_f(m)}. \quad (2.21)$$

If the initial state of the backward process $\tilde{p}_f(m)$ is the final state of the forward process, i.e., $\tilde{p}_f(m) = p_f(m)$ we have $p(\gamma) = e^{\Delta_i s \gamma} \tilde{p}(\tilde{\gamma})$. Using this equality we now evaluate

$$p(\Delta_i s) = \sum_{\gamma} p(\gamma) \delta(\Delta_i s - \Delta_i s \gamma) = e^{\Delta_i s} \sum_{\tilde{\gamma}} \tilde{p}(\tilde{\gamma}) \delta(\Delta_i s + \Delta_i s \tilde{\gamma}) = e^{\Delta_i s} \tilde{p}(-\Delta_i s)$$

where we have also used the fact that $\Delta_i s \tilde{\gamma} = -\Delta_i s \gamma$.

If the reversed process is identical to the forward process, $\tilde{p}(\Delta_i s) = p(\Delta_i s)$, the fluctuation theorem for the entropy production, Eq.(2.18), can be written just with the distribution of the forward process, $p(\Delta_i s) = e^{\Delta_i s} p(-\Delta_i s)$. This is the case in the systems we consider if the driving is time symmetric, $\{H_S(t), V(t)\} = \{H_S(\tau - t), V(\tau - t)\}$ for $0 \leq t < \tau$. A constant H_S and (step) V fulfills this condition. Also it is necessary that the operator that is measured is invariant under the time reversal transformation, guaranteeing a one-to-one correspondence between the forward and backward trajectories, in which there is the same trajectory present in both processes. See Appendix B.

The detailed fluctuation theorem for the entropy production implies the integral fluctuation theorem $\langle e^{-\Delta_i s} \rangle = 1$. This in turns implies that if the average entropy production $\Delta_i S = \langle \Delta_i s \rangle = 0$ vanishes, then $\langle e^{-\Delta_i s} \rangle = e^{\langle -\Delta_i s \rangle}$ and due to the convexity of the exponential this is possible only if $p(\Delta_i s) = \delta(\Delta_i s)$, i.e., the stochastic entropy production does not fluctuate. This was already noticed when we discussed maps with equilibrium states and the fluctuation properties in these states. On the other hand, it implies the opposite for *non-equilibrium* steady state, that is, fluctuations of the stochastic entropy production are necessary to have a positive average entropy production $\Delta_i S = \langle \Delta_i s \rangle > 0$.

2.4.2 Fluctuations of work

Consider now the case where the initial states of the forward and backward processes are canonical, $p_i(n) = e^{-\beta \epsilon_n} / Z_S$ and $\tilde{p}_f(m) = e^{-\beta \epsilon_m} / Z_S$, then Eq.(2.21) gives

$$\frac{p(\gamma)}{\tilde{p}(\tilde{\gamma})} = e^{-\beta(\epsilon_i - \epsilon_j)} e^{-\beta(\epsilon_n - \epsilon_m)} = e^{\beta w_\gamma}. \quad (2.22)$$

One can prove that, if the reversed process is identical to the forward process (see Appendix B), the probability of performing a work w between the initial time with the system in the state $e^{-\beta H_S} / Z_S$ and an arbitrary time (possible after infinite time, when the system reaches the steady state) at which the energy of the system is measured satisfies the fluctuation relation

$$p(w) = p(-w) e^{\beta w}. \quad (2.23)$$

If instead, the reversed process is not the same as the forward process, the work fluctuation theorem reads $p(w) = \tilde{p}(-w) e^{\beta w}$. For thermal maps, whose stationary state is the canonical thermal state, we saw that $p(w) = \delta(w)$ and thus Eq.(2.23) is trivially satisfied. For other maps the canonical thermal state is not necessarily invariant. Thus one can consider the evolution of the system initially prepared in the canonical thermal state towards it's steady state and perform the two-point measurement of the system Hamiltonian to find that the work statistics follows Eq.(2.23). We illustrate later this equality in two interesting situations, a system that undergoes a cyclic process and a system in a non-equilibrium steady state.

2.5 Concatenation of maps

In the previous sections of Chapter 2 we have considered that the process $\rho_S \rightarrow \rho'_S$ is given by a single CPTP map $\rho'_S = \mathcal{E}(\rho_S) = \sum_k M_k \rho_S M_k^\dagger$ with a particular choice for the Kraus operators M_k that allows a thermodynamic interpretation. We will show that the results of the previous sections can be extended to concatenations of maps, providing a richer setup for the study of thermodynamic processes.

One can concatenate CPTP maps acting over a system to describe a sequence of coupled evolution of a system to a heat bath for given lapses of time, as in the repeated scheme of Section 1.2. We generalize the concept of quantum trajectory to concatenations of N maps $\mathcal{E}(\cdot) = \mathcal{E}^{(N)} \dots \mathcal{E}^{(1)}(\cdot)$. Each

$$\mathcal{E}^{(n)}(\cdot) = \sum_k M_k^{(n)} \cdot M_k^{(n)\dagger} \quad (2.24)$$

is a CPTP map and for each we measure a corresponding k_n associated to the process $|i_n\rangle \rightarrow |j_n\rangle$ between eigenstates of the bath. Note that with each map $\mathcal{E}^{(n)}$ a new fresh bath is brought to interaction with the system (see Fig. 1.1 in Section 1.2). For instance, as before we consider the unitary evolution operator $U_n = e^{-i\tau_n(H_S + H_b^n + V^n)}$ with V^n representing the energy coupling between the system and the n th copy of the bath (with Hamiltonian H_b^n) in the time interval $[\sum_{l < n} \tau_l, \sum_{l \leq n} \tau_l]$. We consider V^n constant in this time interval and $V^n = 0$ outside. The Kraus operators are

$$M_{ij}^n = \sqrt{\frac{e^{-\beta \varepsilon_{i_n}}}{Z_b}} \langle j_n | U_n | i_n \rangle, \quad (2.25)$$

where $\{\varepsilon_{i_n}, |i_n\rangle\}$ is the spectrum of H_b^n and $Z_b = \text{Tr} e^{-\beta H_b^n}$. This concatenation of maps is equivalent to the recursion, Eq. (1.15), that is obtained in the repeated interaction scheme. The stochastic heat flow from the bath to the system in this process is given by minus the energy change of the baths $q_\gamma = \sum_n (\varepsilon_{i_n} - \varepsilon_{j_n})$.

As before, we perform a measurement of a system operator A at the beginning and another B at the end of the process. The trajectory is $\gamma = \{n, k_1, \dots, k_N, m\}$ and its probability $p(\gamma) = p(m, k_1, \dots, k_N | n) p_i(n)$ is

$$p(\gamma) = |\langle b_m | M_{k_N}^{(N)} \dots M_{k_1}^{(1)} | a_n \rangle|^2 p_i(n) \quad (2.26)$$

or explicitly in terms of Eq.(2.24) and Eq.(2.25) the probability of a trajectory

$$\gamma = \{a_n; i_1, j_1; \dots; i_N, j_N; b_m\} \quad (2.27)$$

is

$$p(\gamma) = |\langle b_m, j_1 \dots j_N | U_N \dots U_1 | i_1 \dots i_N, a_n \rangle|^2 \frac{e^{-\beta \sum_{n=1}^N \varepsilon_{i_n}}}{Z_b^N} p_i(n) \quad (2.28)$$

With this, the detailed fluctuation theorem can be extended to concatenations of maps. If in the forward process the sequence $\mathcal{E}^{(N)} \dots \mathcal{E}^{(1)}$ acts on an initial state, the backward process is the reversed concatenation of the reversed maps, i.e., $\tilde{\mathcal{E}}^{(1)} \dots \tilde{\mathcal{E}}^{(N)}$, and for a given trajectory

$\gamma = \{n, k_1 \cdots k_N, m\}$ the corresponding backward trajectory is $\tilde{\gamma} = \{\tilde{m}, \tilde{k}_N \cdots \tilde{k}_1, \tilde{n}\}$. The probability of the forward path is given by Eq.(2.26) while for the backward path is given by

$$\tilde{p}(\tilde{\gamma}) = |\langle \tilde{a}_n | \tilde{M}_{k_1}^{(1)} \cdots \tilde{M}_{k_N}^{(N)} | \tilde{b}_m \rangle|^2 \tilde{p}_f(m) \quad (2.29)$$

Because every Kraus operator involved in Eq.(2.29) satisfies Eq.(2.20) one gets

$$\frac{p(\gamma)}{\tilde{p}(\tilde{\gamma})} = e^{-\beta q_\gamma} \frac{p_i(n)}{\tilde{p}_f(m)} \quad (2.30)$$

and as before, considering the initial state of the backward process $\tilde{p}_f(m)$ as the final state of the forward process, i.e., $\tilde{p}_f(m) = p_f(m)$ we have $p(\gamma) = e^{\Delta_i s_\gamma} \tilde{p}(\tilde{\gamma})$. Finally, if the initial states of the forward and backward processes are canonical, $p_i(n) = e^{-\beta \epsilon_n} / Z_S$ and $\tilde{p}_f(m) = e^{-\beta \epsilon_m} / Z_S$, then Eq.(2.30) gives $\frac{p(\gamma)}{\tilde{p}(\tilde{\gamma})} = e^{-\beta q_\gamma} e^{-\beta(\epsilon_n - \epsilon_m)} = e^{\beta w_\gamma}$.

Note that for every iteration of the map there is certain amount of average work, heat and entropy production. These quantities are additive. This means that if we know the average work, heat and/or entropy production for two maps that are composed, the average work, heat and/or entropy production for the total map (the composition) is the sum of the corresponding quantity for each map. For fluctuations this separation is not possible since a projective measurement in the system between one map and another would change the system. The averaged stochastic thermodynamic quantities would not correspond to the mean thermodynamic quantities of the process without measurements.

2.5.1 Thermodynamic cycle

We can illustrate the advantage of considering concatenations of maps by studying a simple thermodynamic cycle. A system starts in the canonical thermal state $\omega_\beta(H_S)$ and then it is driven by a map such as those considered in Section 2.3 where work is performed on the system leaving it in a non-equilibrium state ρ'_S but with the same Hamiltonian H_S . Then we assume that a thermal map brings the system back to the thermal state $\omega_\beta(H_S)$. For such a cycle we have that

$$\Delta E = 0 = W_d + Q_d + Q_r$$

where Q_d and W_d refer respectively to the heat exchanged with the bath, Eq.(2.8), and the work performed on the system, Eq.(2.9), during the driving process $\omega_\beta(H_S) \rightarrow \rho'_S$ and Q_r is the heat exchanged during the final relaxation process $\rho'_S \rightarrow \omega_\beta(H_S)$. Since this is achieved with a thermal map one has $W_r = 0$ and thus $Q_r = \text{Tr}[H_S(\omega_\beta(H_S) - \rho'_S)]$. Also one can check that

$$\Delta S = 0 = \Delta_i S_d + \Delta_i S_r + \beta(Q_d + Q_r)$$

where according to Eq.(2.12) and Eq.(2.16), $\Delta_i S_d = D(\rho'_{\text{tot}} || \rho'_S \otimes \omega_\beta(H_B))$ and $\Delta_i S_r = D(\rho'_S || \omega_\beta(H_S))$, respectively. It also follows that the total entropy production $\Delta_i S_d + \Delta_i S_r = \beta W_d$ is the dissipated work as expected for a isothermal process starting and finishing in equilibrium. We also get $\Delta_i S_d = -D(\rho'_S || \omega_\beta(H_S)) + \beta W_d$ [29].

Now we consider fluctuations. Note that because the initial and final density matrices are Gibbsian, work and entropy production fluctuations are the same,

$$\ln \frac{p(\gamma)}{\tilde{p}(\tilde{\gamma})} = \Delta_i s_\gamma = \Delta s_\gamma - \beta(q_\gamma^d + q_\gamma^r) = \beta \Delta \epsilon_\gamma - \beta(q_\gamma^d + q_\gamma^r) = \beta w_\gamma. \quad (2.31)$$

In the last equation, $q_\gamma^{d,r}$ are the driving and relaxation stochastic heat, respectively.

Usually, the thermal state is achieved asymptotically when a system interacts with a large memoryless heat bath. This thermalization might also be achieved by concatenating (in theory) an infinite sequence of thermal maps, taking the limit $N \rightarrow \infty$ in the process described with Eqs.(2.24) and (2.25). This composition is also a thermal map. In the first example of the next section we show that in practice, this can be done much quicker with just a few maps when the system is small.

2.6 Applications

2.6.1 Single spin in a thermodynamic cycle

Consider a single spin with $H_S = (h/2)\sigma_S^z$, that interacts with thermal spins $\omega_\beta(H_b^n)$, with $H_b^n = (h/2)\sigma_b^z$. Here $\sigma_{S,b}^{x,y,z}$ are the Pauli spin 1/2 operators of the system and bath. The interaction V^1 with the first spin is such that $[H_S + H_b^1, V^1] \neq 0$ and thus if the system spin starts in equilibrium, $\rho_S = \omega_\beta(H_S)$, the interaction with the first spin drives the system out of equilibrium to a state $\mathcal{E}^{(1)}(\omega_\beta(H_S))$. Then for the subsequent interactions we take V^n such that $[H_S + H_b^n, V^n] = 0$ with $n \geq 2$ and thus the corresponding $\{\mathcal{E}^{(n)}\}_{n \geq 2}$ are thermal maps that will bring the system back to the thermal $\omega_\beta(H_S)$ state. This constitutes a thermodynamic cycle for the system with a unitary evolution for the spin plus baths total system. As a consequence, the micro-reversibility principle is valid and Eq.(2.31) is fulfilled (see the next example for details on the time reversal operator). In the left panel of Fig. 2.1 we plot the (Hilbert-Schmidt) distance $D_{HS}(\sigma, \rho) = \|\sigma - \rho\|_{HS}^2 = \text{Tr}[(\sigma - \rho)^2]$ between the state of the system at each step of the concatenation and the thermal state and observe that indeed as N grows thermalization becomes more effective. In the right panel we show work and entropy production probability distributions for the cycle considering that at $N = 7$ thermalization has been achieved ($\|\rho'_S - \omega_\beta(H_S)\|_{HS} < 10^{-5}$). We show in Appendix C that thermal maps do not contribute to work fluctuations, thus we plot work fluctuations of the driving part alone as well as of the full cycle, $p_1 \equiv p_{\text{cycle}}(\beta w) = p_{\text{drive}}(\beta w) = p_{\text{cycle}}(\Delta_i s)$. Note that this does not apply for entropy production, $p_2 \equiv p_{\text{drive}}(\Delta_i s) \neq p_1$.

The numerical calculations can be done straightforwardly due to the fact that at every iteration, the Hilbert space is small: two qubits in this case, one corresponding to the bath and one to the system. The evolution is carried out multiplying the total system-bath density matrix with the unitary evolution operators and partially tracing the resulting matrix. The measurements in the trajectories are simulated numerically, i.e., one do a projective measurement over the system and bath and record the results obtained to define a trajectory, then, comparing these one constructs the stochastic thermodynamic quantities.

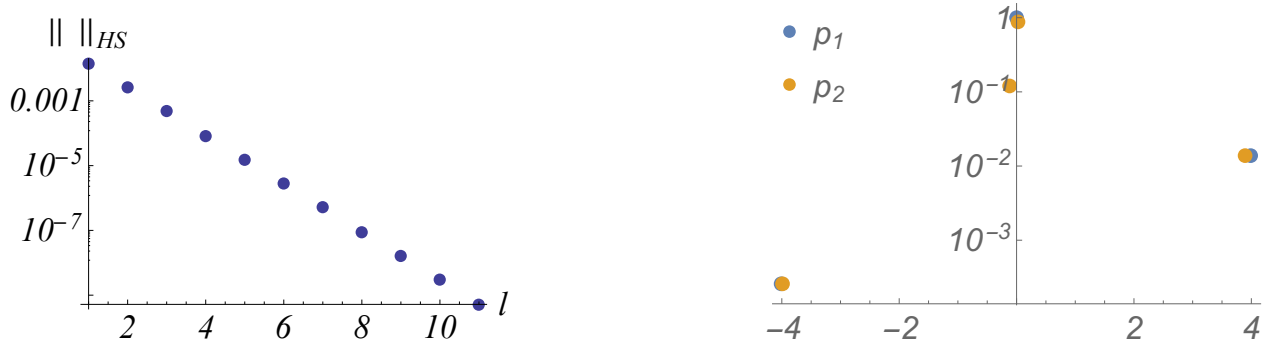


Figure 2.1: Left panel) Hilbert-Schmidt distance between the state of the system at each step of the concatenation and the thermal state. In this concatenation process we take $\tau_1 = 1$, $V^1 = (J_B + 0.3)\sigma_b^x\sigma_S^x + J_B\sigma_b^y\sigma_S^y$, $\tau_n = 4$, $V^n = J_B\sigma_b^x\sigma_S^x + J_B\sigma_b^y\sigma_S^y$ for $n \geq 2$ and the other parameters are $h = 1$, $J_B = 3$, and $\beta = 1$. Right panel) Work and entropy production distributions for the full cycle and the driving alone, $p_1 \equiv p_{\text{drive}}(\beta w) = p_{\text{cycle}}(\beta w) = p_{\text{cycle}}(\Delta_i s) \neq p_2 \equiv p_{\text{drive}}(\Delta_i s)$. The parameters for the plot are the same as in the left panel.

2.6.2 Spin 1/2 chains

We recall the example of the spin chain and its properties discussed in Sec. 1.2.2. We consider a one-dimensional spin 1/2 chain $\vec{\sigma}_1 \cdots \vec{\sigma}_M$ with Hamiltonian H_S interacting through its first site with a spin 1/2 particle with Hamiltonian $H_b = \frac{h}{2}\sigma_b^z$ in a thermal state, $\omega_\beta(H_b)$, where the interaction is given by

$$V = J_B(\sigma_b^x\sigma_1^x + \sigma_b^y\sigma_1^y). \quad (2.32)$$

Here the Pauli operators $\sigma_b^{x,y,z}$ belong to the single bath spin and $\sigma_1^{x,y,z}$ to the first spin of the chain. The unitary evolution for the system plus bath is given by the operator $U = e^{-i\tau(H_S+H_b+V)}$. Micro-reversibility holds if there exist an anti-unitary operator Θ such that $\Theta\tilde{U}\Theta^\dagger = U^\dagger$. For the spin systems we consider below $\Theta = i\sigma_b^x i\sigma_b^y \prod_{n=1}^M (i\sigma_n^x i\sigma_n^y) K$ is a time reversal symmetry operator where K performs the complex conjugation. Note that usually when a system involves a magnetic field one needs to invert the direction of the magnetic field and thus the detailed fluctuation theorem in that case will relate the fluctuations of two different systems. However, for the time reversal operator we consider here that is not the case [41]. The factor $i\sigma^x$ rotates the system in 180° in the x direction, leaving the σ^z terms invariant (see below the Hamiltonians). Replacing H_b in Eq.(2.3) one obtain four Kraus operators M_{ij} with $i, j = \pm$, corresponding to transitions in the bath when $i \neq j$.

Let now the system be an XX spin 1/2 chain with Hamiltonian

$$H_{XX} = \frac{h}{2} \sum_{i=1}^M \sigma_i^z - \sum_{i=1}^{M-1} J_i^x (\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y).$$

The total magnetization is a conserved quantity for the XX spin chain, i.e., $[H_{XX}, H_0] = 0$, with $H_0 = \frac{h}{2} \sum_{i=1}^M \sigma_i^z$ the non-interacting part of the Hamiltonian. Considering the Hamiltonian of the bath H_b and the interaction between the chain and the bath V one finds that the unitary evolution $U = e^{-i\tau(H_{XX}+H_b+V)}$ satisfies $[U, H_0 + H_b] = 0$, thus $\omega_\beta(H_0)$ is an equilibrium state of the non-thermal map with equilibrium \mathcal{E} . In this example the Hamiltonian

is of the form $H_S = H_0 + H_I$ with $[H_0, H_I] = 0$. The stochastic thermodynamics for such a system was discussed in Section 2.3.1. We can see that iterating the map as discussed in Section 2.5, an initial state $\rho_S(0)$ converges to the equilibrium state $\omega_\beta(H_0)$. This is illustrated in Fig. 2.2. The average work, heat and entropy production performed on this process in each interaction are given by Eqs.(2.15), (2.14) and (2.16). Thus the cumulated work is $W = \text{Tr}_S[H_I(\omega_\beta(H_0) - \rho_S(0))]$ and because $\text{Tr}_S[H_I\omega_\beta(H_0)] = 0$ in this example it is simply given by $W = -\text{Tr}_S[H_I\rho_S(0)]$. The cumulated heat is $Q = \text{Tr}_S[H_0(\omega_\beta(H_0) - \rho_S(0))]$ and the cumulated entropy production is $\Delta_i S = D(\rho_S(0)||\omega_\beta(H_0))$. These asymptotic values are indicated in Fig. 2.2, left panel. Concerning the fluctuating properties we showed in Section 2.3.1 that in the equilibrium state $\omega_\beta(H_0)$ the entropy production does not fluctuate but work may fluctuate. This is illustrated in Fig. 2.3, left panel.

Let us now consider the XY spin 1/2 chain with Hamiltonian

$$H_{XY} = \frac{\hbar}{2} \sum_{i=1}^M \sigma_i^z - \sum_{i=1}^{M-1} (J_i^x \sigma_i^x \sigma_{i+1}^x + J_i^y \sigma_i^y \sigma_{i+1}^y).$$

coupled to the bath with Hamiltonian H_b through the same coupling V . For this system the invariant state ρ_{XY} of the map \mathcal{E} is not related to any operator H_0 such that $[U, H_0 + H_b] = 0$. Indeed, the state $\rho_{XY} \otimes \omega_\beta(H_b)$ is not invariant under the unitary evolution and this indicates already that the steady state ρ_{XY} is a NESS. We can see that iterating the map for the XY chain a steady state is reached where a constant amount of work is being performed each time the map is applied and the same for the heat and entropy production. This is illustrated by the constant slopes in the cumulated thermodynamic quantities in Fig. 2.2, right panel. These slopes can be computed but not in terms of the system properties only, they are global quantities. For instance the slope for the entropy production is $D(U\rho_{XY} \otimes \omega_\beta(H_b)U^\dagger || \rho_{XY} \otimes \omega_\beta(H_b))$. In this case the map on the XY spin chain is a map with NESS.

Finally, let us consider some fluctuation properties. In the left panel of Fig. 2.3 we plot the work distribution for the XX spin 1/2 chain in the equilibrium state, where $p(\Delta_i s) = \delta(\Delta_i s)$, but as noted before, even though $\langle w \rangle = 0$, the work fluctuates, i.e., $p(w) \neq \delta(w)$. The work fluctuation relation Eq.(2.23) is illustrated in the right panel of Fig. 2.3 for the XY spin chain.



Figure 2.2: Left panel) For the homogeneous XX spin 1/2 chain with three sites, cumulated average work (dashed-black), heat (dashed-red) and entropy production (dashed-blue) as a function of the iteration number. The corresponding straight lines are the theoretically computed asymptotic values. Right panel) The same quantities for the homogeneous XY spin 1/2 chain with three sites. In both cases the initial density matrix is the Gibbs state $\omega_\beta(H_S)$, which is a non-equilibrium state. The parameters for the plots are: $h = 2$, $J_i^x = J_B = 3$, $\beta = 1.2$ and $\tau = 1$, and $J_i^y = 2$ in the right panel.

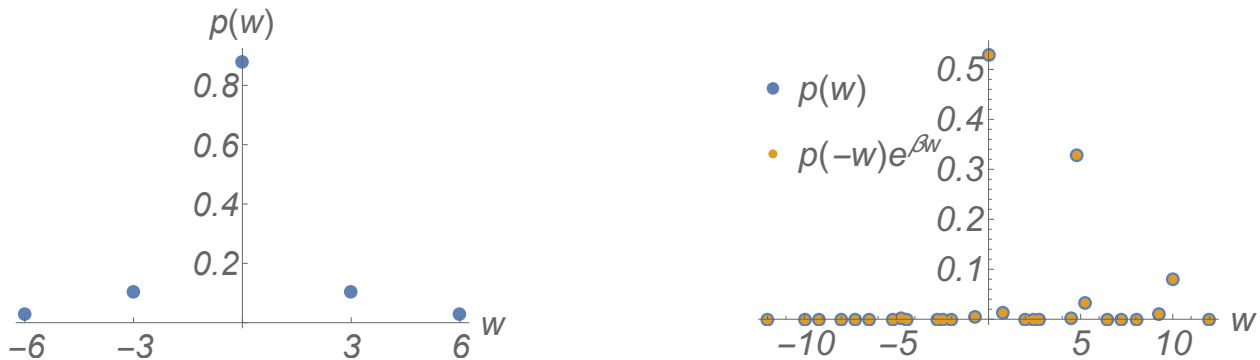


Figure 2.3: Left panel) Work distribution for the XX spin 1/2 chain in the equilibrium state. Right panel) Work fluctuation relation Eq.(2.23) for the XY spin 1/2 chain, starting from the Gibbs state in the forward and backward processes. In both plots we have used a chain of two sites and one map. The parameters for the plots are: $h = 2$, $J_i^x = J_B = 3$, $\beta = 1.2$ and $\tau = 1$, and $J_i^y = 2$ in the right panel. There are a small number of points on both graphics due to the fact that the Hilbert space is discrete and small (2^3), thus work can take some very specified values and many of them have vanishing probability.

Chapter 3

Thermodynamics in the Lindblad limit

3.1 Detailed balance and CPTP maps with equilibrium

A central result of classical thermodynamic and statistical mechanic equilibrium is the principle of detailed balance, which states that [44]

"In the state of equilibrium, every transformation is balanced by its exact opposite or reverse".

The condition of quantum detailed balance for Lindblad type master equations whose stationary state is the equilibrium Gibbs state has been extensively studied [45, 46, 47]. The condition is satisfied if and only if the Lindblad operators and the rates in the equation satisfy some specified relations in relation with the equilibrium state. We will now generalize this condition to the case where the equilibrium state of a Lindblad type master equation is not Gibbisian but $\rho_0 = e^{-\beta H_0}/Z_0$ where $Z_0 = \text{Tr } e^{-\beta H_0}$ and H_0 commutes with the system Hamiltonian, $[H_S, H_0] = 0$. Then we will connect this generalized detailed balance condition to the equilibrium property of a concatenation of CPTP maps with equilibrium (as studied in the previous chapter) in the continuous Lindblad limit.

We consider a Lindblad generator of the form

$$\mathcal{L}(\cdot) = -i[H_S, \cdot] + \sum_r \mathcal{D}_r(\cdot), \quad (3.1)$$

in a finite dimensional Hilbert space \mathcal{H}_S , where $\mathcal{L}_a(\cdot) \equiv -i[H_S, \cdot]$ is the unitary part of the dynamics and $\mathcal{L}_s(\cdot) \equiv \sum_r \mathcal{D}_r(\cdot)$ is the dissipation, with

$$\mathcal{D}_r(\cdot) = \gamma_r [L_r \cdot L_r^\dagger - \frac{1}{2} \{L_r^\dagger L_r, \cdot\}]. \quad (3.2)$$

We will assume that \mathcal{L} has a positive invariant state $\rho_0 > 0$ and that there is no time dependence in the generator.

The dual \mathcal{L}^* of the Lindbladian \mathcal{L} acts on the observables in the Heisenberg picture. It is defined by

$$\begin{aligned}\mathrm{Tr}[Ae^{\mathcal{L}t}(\rho)] &= \mathrm{Tr}[e^{\mathcal{L}^*t}(A)\rho] \\ \mathrm{Tr}[A\mathcal{L}(\rho)] &= \mathrm{Tr}[\mathcal{L}^*(A)\rho],\end{aligned}\tag{3.3}$$

for any observable A (we consider only bounded observables). Thus we have that $\mathcal{L}^* = \mathcal{L}_a^* + \mathcal{L}_s^*$ is given by

$$\mathcal{L}^*(\cdot) = i[H_S, \cdot] + \sum_r L_r^\dagger \cdot L_r - \frac{1}{2}\{L_r^\dagger L_r, \cdot\},\tag{3.4}$$

with $\mathcal{L}_a^*(\cdot) = i[H_S, \cdot]$ and \mathcal{L}_s^* the remaining part.

The generator \mathcal{L} satisfies the quantum generalization of the detailed balance condition [45] with respect to ρ_0 if

$$\mathcal{L}_a(\rho_0) = 0\tag{3.5}$$

$$\mathcal{L}_s(A\rho_0) = \mathcal{L}_s^*(A)\rho_0\tag{3.6}$$

for every A .

The property that connects the detailed balance condition as we have stated it above, with the sentence of Prigogine at the beginning of this chapter is that when H_0 is non-degenerated (and H_S as well), the diagonal terms in the energy representation of ρ_0 are disconnected from the coherences, and their evolution can be described with a Pauli equation

$$\frac{d}{dt}p_l = \sum_k W_{lk}p_k - W_{kl}p_l,\tag{3.7}$$

where $\rho_0 = \sum_l p_l |\epsilon_l\rangle \langle \epsilon_l|$. The coefficients satisfy detailed balance in the classical sense,

$$W_{lk}e^{-\beta\epsilon_k} = W_{kl}e^{-\beta\epsilon_l}.\tag{3.8}$$

We will prove the following equivalence only in the right direction (\Rightarrow) since the other way is straightforward.

Theorem. If and only if \mathcal{L} is a generator of a Lindblad equation of the form Eq.(3.1) and satisfies the generalized detailed balance condition with respect to $\rho_0 = e^{-\beta H_0}/Z_0$ where $Z_0 = \mathrm{Tr}[e^{-\beta H_0}]$ and $[H_S, H_0] = 0$, then the dissipator is of the form

$$\mathcal{L}_s(\cdot) = \sum_r \gamma_r \left[L_r \cdot L_r^\dagger - \frac{1}{2}\{L_r^\dagger L_r, \cdot\} + \omega_r^{-1} \left(L_r^\dagger \cdot L_r - \frac{1}{2}\{L_r L_r^\dagger, \cdot\} \right) \right]\tag{3.9}$$

and the Lindblad operators are eigenoperators of $[H_0, \cdot]$,

$$[H_0, L_r] = -\frac{1}{\beta} \ln \omega_r L_r\tag{3.10}$$

$$[H_0, L_r^\dagger] = \frac{1}{\beta} \ln \omega_r L_r^\dagger.\tag{3.11}$$

Remark I. If the generalization of the detailed balance is fulfilled, choosing A in Eq. (3.6) as the identity gives $\mathcal{L}_s(\rho_0) = 0$, thus ρ_0 is an invariant state. Detailed balance condition is stronger than just having an invariant state.

Remark II. If Eq.(3.5) is satisfied, we have

$$\mathcal{L}_a(A\rho_0) = \mathcal{L}_a(A)\rho_0, \quad (3.12)$$

$$\mathcal{L}_a(\rho_0 A) = \rho_0 \mathcal{L}_a(A), \quad (3.13)$$

$$\mathcal{L}_a^*(A\rho_0) = \mathcal{L}_a^*(A)\rho_0, \quad (3.14)$$

$$\mathcal{L}_a^*(\rho_0 A) = \rho_0 \mathcal{L}_a^*(A). \quad (3.15)$$

Remark III.

$$[\mathcal{L}(A)]^\dagger = \mathcal{L}(A^\dagger), \quad (3.16)$$

$$[\mathcal{L}^*(A)]^\dagger = \mathcal{L}^*(A^\dagger) \quad (3.17)$$

Remark IV.

$$\text{Tr}[\mathcal{L}(A)B] = \text{Tr}[A\mathcal{L}^*(B)]. \quad (3.18)$$

Remark V. The generalized detailed balance condition can be rewritten in the following way. Defining the scalar product $\langle A|B\rangle \equiv \text{Tr}[\rho_0 A^\dagger B]$, the condition can be restated as

$$\begin{aligned} \langle \mathcal{L}_a^*(A)|B\rangle &= -\langle A|\mathcal{L}_a^*(B)\rangle \\ \langle \mathcal{L}_s^*(A)|B\rangle &= \langle A|\mathcal{L}_s^*(B)\rangle. \end{aligned} \quad (3.19)$$

Proof. From Eq.(3.15) and the definition of \mathcal{L}_a^* we have that $\rho_0 \mathcal{L}_a^*(A) = \mathcal{L}_a^*(\rho_0 A) = -\mathcal{L}_a(\rho_0 A)$. Thus,

$$\langle \mathcal{L}_a^*(A)|B\rangle = \text{Tr}[\rho_0 \mathcal{L}_a^*(A^\dagger)B] = -\text{Tr}[\mathcal{L}_a(\rho_0 A^\dagger)B] = -\text{Tr}[\rho_0 A^\dagger \mathcal{L}_a^*(B)] = -\langle A|\mathcal{L}_a^*(B)\rangle. \quad (3.20)$$

On the other hand, using Eq. (3.6),

$$\langle \mathcal{L}_s^*(A)|B\rangle = \text{Tr}[\rho_0 \mathcal{L}_s^*(A^\dagger)B] = \text{Tr}[\mathcal{L}_s(B\rho_0)A^\dagger] = \text{Tr}[\mathcal{L}_s^*(B)\rho_0 A^\dagger] = \text{Tr}[\rho_0 A^\dagger \mathcal{L}_s^*(B)] = \langle A|\mathcal{L}_s^*(B)\rangle. \quad (3.21)$$

Note that this could be thought as \mathcal{L}^* being an operator in the extended space where superoperators become operators and operators become states with the scalar product defined as before. In this way,

$$\langle \mathcal{L}_a^* A|B\rangle = \langle A|\mathcal{L}_a^{*\dagger} B\rangle = -\langle A|\mathcal{L}_a^* B\rangle \quad (3.22)$$

$$\langle \mathcal{L}_s^* A|B\rangle = \langle A|\mathcal{L}_s^{*\dagger} B\rangle = \langle A|\mathcal{L}_s^* B\rangle, \quad (3.23)$$

thus, $\mathcal{L}_a^* = -\mathcal{L}_a^{*\dagger}$ is anti-hermitian and $\mathcal{L}_s^* = \mathcal{L}_s^{*\dagger}$ is hermitian. In general, this can be written compactly as

$$\mathcal{L}^{*\dagger} A = (\mathcal{L} A \rho_0) \rho_0^{-1}. \quad (3.24)$$

We define the superoperator $\Phi : \mathcal{B}(\mathcal{H}_S) \rightarrow \mathcal{B}(\mathcal{H}_S)$, $\Phi(A) = \rho_0 A \rho_0^{-1}$. We have that $\Phi \mathcal{L}^* = \mathcal{L}^* \Phi$.

Proof:

$$\begin{aligned}
\langle \mathcal{L}^*(\Phi(A)), B \rangle &= \text{Tr}[\rho_0 \mathcal{L}^*(\rho_0^{-1} A^\dagger \rho_0) B] \\
&= \text{Tr}[\mathcal{L}(B \rho_0) \rho_0^{-1} A^\dagger \rho_0] \\
&= \text{Tr}[\mathcal{L}^{*\dagger}(B) A^\dagger \rho_0] \\
&= \text{Tr}[\mathcal{L}^*(A^\dagger) \rho_0 B] \\
&= \text{Tr}[\rho_0 \rho_0^{-1} \mathcal{L}^*(A^\dagger) \rho_0 B] \\
&= \text{Tr}[\rho_0 [\rho_0 \mathcal{L}^*(A) \rho_0^{-1}]^\dagger B] \\
&= \text{Tr}[\rho_0 [\Phi(\mathcal{L}^*(A))]^\dagger B] \\
&= \langle \Phi(\mathcal{L}^*(A)), B \rangle.
\end{aligned} \tag{3.25}$$

Φ has the following properties,

- a) $\Phi^\dagger = \Phi$. *Proof:* $\langle \Phi A, B \rangle = \text{Tr}[\rho_0 \rho_0^{-1} A^\dagger \rho_0 B] = \text{Tr}[A^\dagger \rho_0 B] = \text{Tr}[\rho_0 A^\dagger \rho_0 B \rho_0^{-1}] = \langle A, \Phi B \rangle$.
- b) $\Phi > 0$. *Proof:* $\langle A, \Phi A \rangle = \text{Tr}[\rho_0 A^\dagger \rho_0 A \rho_0^{-1}] = \text{Tr}[\rho_0 A A^\dagger] > 0$, $\forall A \in \mathcal{B}(\mathcal{H})$, $A \neq 0$. Note that the last step is due to $\text{Tr}[\rho_0 A A^\dagger] = \sum_n p_n |c_{nk}|^2 > 0$, where $\rho_0 = \sum_n p_n |n\rangle \langle n|$ with $p_n > 0$ and $c_{nk} = \langle n| A |k\rangle$.
- c) $\Phi A = \alpha A \Rightarrow \Phi A^\dagger = \alpha^{-1} A^\dagger$, where $\alpha = \langle A^\dagger, A^\dagger \rangle / \langle A, A \rangle$. *Proof:* $\Phi(A^\dagger) = (\rho^{-1} A \rho_0)^\dagger = [\Phi^{-1}(A)]^\dagger = (\alpha^{-1} A)^\dagger = \alpha^{-1} A^\dagger$. And $\langle A^\dagger, A^\dagger \rangle = \text{Tr}[\rho_0 A A^\dagger] = \text{Tr}[\rho_0 A \rho_0^{-1} \rho_0 A^\dagger] = \alpha \text{Tr}[A \rho_0 A^\dagger] = \alpha \langle A, A \rangle$.

Proof of the Theorem: First, note that $\mathcal{L}_s^* A = \Phi \mathcal{L}_s^* \Phi^{-1} A$, thus

$$\mathcal{L}_s^*(A) = \sum_r \gamma_r [L_r^\dagger A L_r - \frac{1}{2} \{L_r^\dagger L_r, A\}] \tag{3.26}$$

must be equal for every A to

$$\Phi(\mathcal{L}_s^*(\Phi^{-1}(A))) = \sum_r \gamma_r [\Phi(L_r^\dagger) A \Phi(L_r) - \frac{1}{2} \{\Phi(L_r^\dagger L_r), A\}] \tag{3.27}$$

Comparing both equations we have that L_r is an eigenoperator of Φ . We write $\Phi L_r = \omega_r L_r$, $\Phi L_r^\dagger = \omega_r^{-1} L_r^\dagger$.

Second, we have that $\mathcal{L}_s^*(A) = \mathcal{L}_s(A \rho_0) \rho_0^{-1}$. Thus, Eq.(3.26) must be equal for every A to

$$\mathcal{L}_s^*(A \rho_0) \rho_0^{-1} = \sum_r \gamma_r [L_r A \Phi(L_r^\dagger) - \frac{1}{2} \{L_r^\dagger L_r, A\}] \tag{3.28}$$

$$= \sum_r \gamma_r [\omega_r^{-1} L_r A L_r^\dagger - \frac{1}{2} \{L_r^\dagger L_r, A\}] \tag{3.29}$$

This means there must exist an adjoint term in the summation given by $\gamma_r^{\text{adj}}[L_r A L_r^\dagger - 1/2\{L_r L_r^\dagger, A\}]$. We thus have

$$\mathcal{L}_s^*(A) = \sum_r \gamma_r [L_r^\dagger A L_r - \frac{1}{2}\{L_r^\dagger L_r, A\}] + \gamma_r^{\text{adj}} [L_r A L_r^\dagger - \frac{1}{2}\{L_r L_r^\dagger, A\}] \quad (3.30)$$

$$= \mathcal{L}_s^*(A \rho_0) \rho_0^{-1} \quad (3.31)$$

$$= \sum_r \gamma_r [L_r A \Phi(L_r^\dagger) - \frac{1}{2}\{L_r^\dagger L_r, A\}] + \gamma_r^{\text{adj}} [L_r^\dagger A \Phi(L_r) - \frac{1}{2}\{L_r L_r^\dagger, A\}] \quad (3.32)$$

$$= \sum_r \gamma_r [\omega_r^{-1} L_r A L_r^\dagger - \frac{1}{2}\{L_r^\dagger L_r, A\}] + \gamma_r^{\text{adj}} [\omega_r L_r^\dagger A L_r - \frac{1}{2}\{L_r L_r^\dagger, A\}]. \quad (3.33)$$

Comparing we obtain that $\gamma_r^{\text{adj}} = \omega_r^{-1} \gamma_r$, i.e., Eq. (3.9).

Note that $\rho_0 L_r \rho_0^{-1} = e^{-\beta H_0} L_r e^{\beta H_0} = \omega_r L_r$ is equivalent to Eq.(3.10). In fact, defining the function

$$F(x) = e^{-x\beta H_0} L_r e^{x\beta H_0} = \sum_{n=0}^{\infty} \frac{F_n}{n!} x^n, \quad (3.34)$$

with some unknown coefficients F_n in the series expansion, we have that

$$\frac{dF(x)}{dx} = -\beta [H_0, F(x)]. \quad (3.35)$$

Replacing the series expansion in both sides we get

$$\sum_{n=1}^{\infty} \frac{F_n}{(n-1)!} x^{n-1} = \sum_{n=0}^{\infty} \frac{F_{n+1}}{n!} x^n = \sum_{n=0}^{\infty} -\beta \frac{1}{n!} [H_0, F_n] x^n. \quad (3.36)$$

Equating equal powers of x we obtain the recursion $F_{n+1} = -\beta [H_0, F_n]$, with $F_0 = L_r$. Now, since $F(x=1) = \omega_r L_r$, we have that

$$\sum_n \frac{(-\beta)^n}{n!} \text{Comm}^{n+1}(H_0, L_r) = \omega_r L_r, \quad (3.37)$$

where $\text{Comm}^1(H_0, L_r) = [H_0, L_r]$, $\text{Comm}^2(H_0, L_r) = [H_0, [H_0, L_r]]$, etc. Thus, $[H_0, L_r] = -\frac{1}{\beta} \ln \omega_r L_r$. Analogously, for L_r^\dagger we have $[H_0, L_r^\dagger] = \frac{1}{\beta} \ln \omega_r L_r^\dagger$. This ends the proof. We remark that this is actually an equivalence, but the proof of the implication in the other direction (\Leftarrow) is straightforward. \blacksquare

Suppose that for a particular generator we do not have a analytic expression for the invariant state. If the Lindblad operators $\{L_r\}$ are local (boundary driven Lindblad equation), in the sense that they act on a subspace D of the N -dimensional Hilbert space, i.e., $L_r = L_r^{\text{loc}(D)} \otimes \mathbb{1}_{N-D}$, it is possible that the generator has detailed balance (checked numerically) with respect to an invariant state different from Gibbs, $\rho_0 \neq e^{-\beta H_S}/Z$. If this is the case and if the invariant state is reached from a positive initial condition, $\rho^{\text{ini}} > 0$, then ρ_0 can be expressed as $e^{-\beta H_0}/Z_0$ since \mathcal{L} conserves the positivity. It would be useful to find H_0 and β , but unfortunately this is not possible since the only information we have is

$$[H_S, \rho_0] = 0 \quad (3.38)$$

$$[\rho_0, L_r] = \omega_r L_r \quad (3.39)$$

$$[\rho_0, L_r^\dagger] = \omega_r^{-1} L_r^\dagger, \quad (3.40)$$

and even though we know the invariant state can be expressed as $\rho_0 = e^{-\beta H_0}/Z_0$ and so we can rewrite these expressions as

$$[H_S, \ln \rho_0] = [H_S, -\beta H_0] = 0 \quad (3.41)$$

$$[\ln \rho_0, L_r] = [-\beta H_0, L_r] = \ln \omega_r L_r \quad (3.42)$$

$$[\ln \rho_0, L_r^\dagger] = [-\beta H_0, L_r^\dagger] = -\ln \omega_r L_r^\dagger, \quad (3.43)$$

all we could solve for is the product βH_0 , since changing $\beta \rightarrow \beta' = \beta/\alpha$ and $H_0 \rightarrow H'_0 = \alpha H_0$ with any constant number α gives the same equations. Only when the equilibrium state is Gibbsian, $H_S = H_0$, then the inverse temperature can be obtained from Eqs.(3.42) or (3.43). We will assume then that β can be fixed arbitrarily, which makes sense if one thinks of it just as a measure of the scale of the energies.

We will now connect the generalized quantum detailed balance principle for the Lindblad evolution to the equilibrium property of a CPTP map when a concatenation of them is considered. To do so, we will first recall the CPTP map \mathcal{E} we are interested in, Eq.(2.2), i.e.,

$$\rho'_S = \mathcal{E}(\rho_S) = \text{Tr}_B[U \rho_S \otimes \omega_\beta(H_B) U^\dagger], \quad (3.44)$$

where we know that \mathcal{E} is an equilibrium map if there is a stationary state $\pi = e^{-\beta H_0}/Z_0$ with $[H_S, H_0] = 0$ and $[V, H_0 + H_B] = 0$. We first note that scaling the coupling as $V = v/\sqrt{\tau}$, the map \mathcal{E} can be written up to order τ as

$$\mathcal{E}^\tau(\rho_S) = \rho_S - i\tau[H_S, \rho_S] + \tau \sum_{ij} \frac{e^{-\beta \varepsilon_i}}{Z_B} \left(\langle \varepsilon_j | v | \varepsilon_i \rangle \rho_S \langle \varepsilon_i | v | \varepsilon_j \rangle - \frac{1}{2} \{ \langle \varepsilon_i | v | \varepsilon_j \rangle \langle \varepsilon_j | v | \varepsilon_i \rangle, \rho_S \} \right), \quad (3.45)$$

where $H_B |\varepsilon_i\rangle = \varepsilon_i |\varepsilon_i\rangle$. Writing $M_{ij} = \langle \varepsilon_j | v | \varepsilon_i \rangle$ (v is hermitian) we get a dissipator

$$\tau \sum_{ij} \frac{e^{-\beta \varepsilon_i}}{Z_B} \left(M_{ij} \rho_S M_{ij}^\dagger - \frac{1}{2} \{ M_{ij}^\dagger M_{ij}, \rho_S \} \right) \quad (3.46)$$

$$= \tau \sum_{i < j} \frac{e^{-\beta \varepsilon_i}}{Z_B} \left[M_{ij} \rho_S M_{ij}^\dagger - \frac{1}{2} \{ M_{ij}^\dagger M_{ij}, \rho_S \} + e^{\beta(\varepsilon_i - \varepsilon_j)} \left(M_{ij}^\dagger \rho_S M_{ij} - \frac{1}{2} \{ M_{ij} M_{ij}^\dagger, \rho_S \} \right) \right] \\ + \tau \frac{e^{-\beta \varepsilon_i}}{Z_B} \left(M_{ii} \rho_S M_{ii}^\dagger - \frac{1}{2} \{ M_{ii}^\dagger M_{ii}, \rho_S \} \right). \quad (3.47)$$

Since $[H_0, v] = [v, H_B]$, we have that

$$[H_0, M_{ij}] = (\varepsilon_i - \varepsilon_j) M_{ij} \quad (3.48)$$

$$[H_0, M_{ij}^\dagger] = -(\varepsilon_i - \varepsilon_j) M_{ij}^\dagger. \quad (3.49)$$

Note that if we consider the the labels $\{ij\}$ as one label, $r = ij$, then we can identify the Lindblad operators $L_r = M_{ij}$ and the coefficients $\omega_r = e^{\beta(\varepsilon_j - \varepsilon_i)}$. The conditions Eqs.(3.10) and (3.11) are satisfied. Note that the second line of Eq.(3.47) can be rewritten as

$$\tau \frac{1}{2} \frac{e^{-\beta \varepsilon_i}}{Z_B} \left(M_{ii} \rho_S M_{ii}^\dagger - \frac{1}{2} \{ M_{ii}^\dagger M_{ii}, \rho_S \} + M_{ii}^\dagger \rho_S M_{ii} - \frac{1}{2} \{ M_{ii} M_{ii}^\dagger, \rho_S \} \right), \quad (3.50)$$

thus Eq.(3.47) is of the form Eq.(3.9) with $\gamma_r = e^{-\beta\epsilon_i}/Z_B$ when $i \neq j$ and $\gamma_r = e^{-\beta\epsilon_i}/2Z_B$ when $i = j$. Finally, the equivalence between the equilibrium condition for a repeated interaction generated by a concatenation of CPTP maps of the form Eq.(3.44) and the condition for the quantum detailed balance of the Lindblad form is completed noting that the Lindblad generator can be written in its infinitesimal form as $\mathcal{L}^\tau \equiv \mathbb{1} + \tau\mathcal{L} = \mathcal{E}^\tau$, where $\rho_S(t + \tau) = \mathcal{L}^\tau(\rho_S(t))$.

If our Lindblad equation of interest has detailed balance with a positive invariant non-Gibbsian equilibrium state, i.e., $\rho_0 \neq \omega_\beta(H_S)$, then it is trivial to find a repeated interaction that generates that continuous evolution in the Lindblad limit. In this case, the thermodynamic quantities for CPTP maps which are simplified due to an equilibrium, Eqs.(2.14), (2.15) and (2.16), can be written in the following way in the Lindblad limit, without needing explicit knowledge of the particular form of H_B and the coupling V :

$$\dot{Q}(t) = \text{Tr}[H_0\mathcal{L}(\rho(t))] \quad (3.51)$$

$$\dot{W}(t) = \text{Tr}[(H - H_0)\mathcal{L}(\rho(t))] \quad (3.52)$$

$$\dot{S}_i(t) = -\text{Tr}[\mathcal{L}(\rho(t)) \ln \rho(t)] - \beta\dot{Q}. \quad (3.53)$$

We would like to emphasize that there is no need of actually finding the repeated interaction that generates a particular Lindblad equation when it has detailed balance. One can just use Eqs.(3.51), (3.52) and (3.53) to make a consistent thermodynamic analysis of any far from equilibrium process (note that since $\mathcal{L}(\rho_0) = 0$ in the equilibrium state the three thermodynamic quantities vanish), just with the Lindblad equation. Anyhow, in the following section we show some examples where we start from Lindblad equations with and without detailed balance and obtain the repeated interaction scheme that generates them in the Lindblad limit.

We should finally remark that if the equilibrium state for which detailed balance is valid is Gibbsian, $\rho_0 = \omega_\beta(H_S) = e^{-\beta H_S}/Z_S$, like in the standard Lindblad equations in the weak coupling regime, the Lindblad operators are global (they act on the full system) and our analysis is still correct. In that case, $\dot{W} = 0$ according to Eqs.(3.52), while Eqs.(3.51) and Eq.(3.53) give the standard definitions used for the heat flux, $\dot{Q}(t) = \text{Tr}[H_S\dot{\rho}_S]$, and for the entropy production rate $\dot{S}_i(t) = -(d/dt)D[\rho(t)||\omega_\beta(H_S)]$, in the weak-coupling regime.

3.2 Examples

3.2.1 Spin 1/2 chains

We have already investigated the properties of the XX and XY spin chains in the repeated interaction and took the Lindblad limit to obtain the dissipator Eq.(1.25). We will now show how to proceed in the reversed way: starting from a Lindblad equation for the spin chain we obtain a repeated interaction that generates it.

Suppose we know $H_0 = (\hbar/2) \sum_i \sigma_i^z$ is a conserved quantity of the system, $[H_S, H_0] = 0$, and we would like to construct a boundary Lindblad equation with detailed balance with

respect to $\rho_0 = \omega_\beta(H_0) = e^{-\beta H_0}/Z_0$. A boundary driven Lindblad equation can be of the form

$$\partial_t \rho_S = -i[H_S, \rho_S] + \gamma_+ \left[\sigma_1^+ \rho_S \sigma_1^- - \frac{1}{2} \{ \sigma_1^- \sigma_1^+, \rho_S \} + \omega_+^{-1} \left(\sigma_1^- \rho_S \sigma_1^+ - \frac{1}{2} \{ \sigma_1^+ \sigma_1^-, \rho_S \} \right) \right], \quad (3.54)$$

with $H_S = H_{XX} = \frac{\hbar}{2} \sum_{i=1}^N \sigma_i^z - \sum_{i=1}^{N-1} J_i^x (\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y)$ and where $\sigma_i^\pm = \sigma_i^x \pm i \sigma_i^y$. We require for detailed balance that the coefficient ω_+^{-1} satisfies the following relations:

$$[H_0, \sigma_1^+] = -\frac{1}{\beta} \ln \omega_+ \sigma_1^+ \quad (3.55)$$

$$[H_0, \sigma_1^-] = \frac{1}{\beta} \ln \omega_+ \sigma_1^- \quad (3.56)$$

Calculating the commutators we readily obtain that $\omega_+ = e^{-\beta h}$. The other coefficient, γ_+ , is arbitrary for the moment but later we will note that it must be bounded. Now we ask ourselves how must the coupling v between the system and the bath be so that we obtain the Lindblad operators σ_1^\pm with $M_{ij} = \langle \varepsilon_j | v | \varepsilon_i \rangle$. A straightforward solution is

$$v = \sigma_b^+ \sigma_1^- + \sigma_b^- \sigma_1^+ \quad (3.57)$$

for a two level bath, since $\langle + | v | - \rangle = \sigma_1^-$ and $\langle - | v | + \rangle = \sigma_1^+$, where $|\pm\rangle$ are the bath energy eigenstates $|\varepsilon_i\rangle$. Thus we know from this that $H_B \propto \sigma_b^z$. Comparing Eq.(3.47) with the dissipator of Eq.(3.54) we note that

$$\gamma_+ = \frac{e^{-\beta \varepsilon_+}}{Z_B} \quad (3.58)$$

where $H_B |+\rangle = \varepsilon_+ |+\rangle$. Writing the bath Hamiltonian as $H_B = h_b \sigma_b^z$ we obtain $\gamma_+ = (1 - \tanh(\beta h_b))/2$, thus h_b can be determined from γ_+ if and only if $-1 \leq 1 - 2\gamma_+ \leq 1$. There is yet another constraint. Since $[v, H_0 + H_B] = 0$, we require $h = h_b$, so γ_+ and ω_+ are fully determined once one fix the inverse temperature β .

In the case of the XY ($H_{XY} = \frac{\hbar}{2} \sum_{i=1}^N \sigma_i^z - \sum_{i=1}^{N-1} J_i^x \sigma_i^x \sigma_{i+1}^x + J_i^y \sigma_i^y \sigma_{i+1}^y$) spin chain one does not have an operator H_0 which commutes with H_{XY} , so the detailed balance condition is not fulfilled and we do not have Eqs.(3.10) and (3.11). However, one can obtain the repeated interaction that generates a Lindblad evolution like Eq.(3.54) for the XY spin chain without detailed balance making use of another system which has detailed balance, in this case, the XX spin chain. Actually, choosing the same coefficients for the dissipator as before for the XX spin chain one obtains a repeated interaction of a CPTP map \mathcal{E} with a NESS for the XY chain as the one considered in Section 2.6.2.

3.2.2 The smallest possible refrigerator

In [48, 31] a refrigerator composed of three qubits connected each one to a different bath is studied. A Lindblad equation is given with intuitive arguments. A simple reset model

is used where with probability p_i per time τ each qubit may reset to a Gibbs state $\omega_{\beta_i}(H_i)$ where $H_i = E_i |1\rangle_i \langle 1|_i$ is the Hamiltonian of the i -qubit with $|1\rangle_i$ its excited state and β_i is the inverse temperature of the bath connected to the qubit i . A non-unitary process occurs in the time τ given by

$$\rho_S \rightarrow \sum_{i=1}^3 \tau p_i \omega_{\beta_i}(H_i) \otimes \text{Tr}_i(\rho_S) + (1 - \tau p_i) \rho_S. \quad (3.59)$$

Baths with temperatures T_C , T_R and T_H are connected to qubits 1,2 and 3, respectively, where C stands for “cold”, R for “room”, and H for “hot”. There is a free Hamiltonian $H_0 = \sum_{i=1}^3 E_i \Pi_i$ where $\Pi_i = |1\rangle_i \langle 1|_i$ is the projector to the excited state of the qubit i , and a interacting Hamiltonian $H_{\text{int}} = g(|101\rangle \langle 010| + |010\rangle \langle 101|)$ which couples the three qubits. The idea is that constraining the energies to $E_2 = E_1 + E_3$ the interaction couples states of equal energy. If the evolution were unitary, nothing will change since the populations of $|101\rangle$ and $|010\rangle$ would change with equal probability, but choosing $T_R < T_H$ the state $|010\rangle$ is preferred which brings the qubit 1 to the ground state, thus energy is constantly being pumped from the cold bath because it needs to give energy to thermalize the first qubit. The result is that qubit 1 reaches a stationary effective temperature lower than that of its bath, $T_1^s < T_C$.

In the limit $\tau \rightarrow 0$ a Lindblad equation (we will show in a moment that it can be rewritten in Lindblad form) is obtained:

$$\partial_t \rho_S = -i[H_0 + H_{\text{int}}, \rho_S] + \sum_i p_i (\omega_{\beta_i}(H_i) \otimes \text{Tr}_i(\rho_S) - \rho_S). \quad (3.60)$$

It is argued that the inclusion of H_{int} would require modifications to the dissipator, but in the limit $g \rightarrow 0$, $p_i \rightarrow 0$ and g/p_i constant, the corrections are of order gp_i . This refrigerator can reach Carnot efficiency, which is calculated in terms of heats only because there is no work, $\eta = \dot{Q}_C / \dot{Q}_H = E_1 / E_3 \leq (1 - \frac{T_R}{T_H}) / (\frac{T_R}{T_C} - 1) = \eta^C$.

A later article [49] argues that this local dissipator (in the sense that Lindblad operators act locally in a subspace of the system) might not be realistic. They do modifications to the Lindblad equation and obtain a lower constraint on the efficiency. We would now like to argue that Eq.(3.60) can be obtained from a repeated interaction without any assumptions on g or p_i and that the efficiency must be modified because it requires work.

We first rewrite Eq.(3.60) in Lindblad form. We will for the moment write ρ_S as ρ just to simplify the notation. We define $r_i = \langle 0|_i \omega_{\beta_i}(H_i) |0\rangle_i$ and $\bar{r}_i = \langle 1|_i \omega_{\beta_i}(H_i) |1\rangle_i$. Thus,

$$\begin{aligned} \tau_i \text{Tr}_i \rho &= (r_i |0\rangle \langle 0|_i + \bar{r}_i |1\rangle \langle 1|_i) \otimes (\langle 0| \rho |0\rangle_i + \langle 1| \rho |1\rangle_i) \\ &= r_i |0\rangle \langle 0|_i \rho |0\rangle \langle 0|_i + r_i |0\rangle \langle 1|_i \rho |1\rangle \langle 0|_i + \bar{r}_i |1\rangle \langle 0|_i \rho |0\rangle \langle 1|_i + \bar{r}_i |1\rangle \langle 1|_i \rho |1\rangle \langle 1|_i \\ &= r_i (\sigma_i^- \sigma_i^+) \rho (\sigma_i^- \sigma_i^+) + r_i \sigma_i^- \rho \sigma_i^+ + \bar{r}_i \sigma_i^+ \rho \sigma_i^- + \bar{r}_i (\sigma_i^+ \sigma_i^-) \rho (\sigma_i^+ \sigma_i^-). \end{aligned} \quad (3.61)$$

Also, since $r_i + \bar{r}_i = 1$, we have that

$$\rho = r_i \rho + \bar{r}_i \rho = r_i \frac{1}{2} \left\{ \mathbb{1}, \rho \right\} + \bar{r}_i \frac{1}{2} \left\{ \mathbb{1}, \rho \right\} = r_i \frac{1}{2} \left\{ (\sigma_i^+ \sigma_i^-) + (\sigma_i^- \sigma_i^+), \rho \right\} + \bar{r}_i \frac{1}{2} \left\{ (\sigma_i^+ \sigma_i^-) + (\sigma_i^- \sigma_i^+), \rho \right\}. \quad (3.62)$$

Adding this last two terms we obtain

$$\begin{aligned}
p_i(\tau_i \text{Tr} - \rho) = & p_i \left[\bar{r}_i \left(\sigma_i^+ \rho \sigma_i^- - \frac{1}{2} \{ (\sigma_i^- \sigma_i^+), \rho \} \right) + r_i \left(\sigma_i^- \rho \sigma_i^+ - \frac{1}{2} \{ (\sigma_i^+ \sigma_i^-), \rho \} \right) \right. \\
& \left. + \bar{r}_i \left((\sigma_i^+ \sigma_i^-) \rho (\sigma_i^+ \sigma_i^-) - \frac{1}{2} \{ (\sigma_i^+ \sigma_i^-), \rho \} \right) + r_i \left((\sigma_i^- \sigma_i^+) \rho (\sigma_i^- \sigma_i^+) - \frac{1}{2} \{ (\sigma_i^- \sigma_i^+), \rho \} \right) \right], \tag{3.63}
\end{aligned}$$

$$\tag{3.64}$$

where it was used that $(\sigma_i^\pm \sigma_i^\mp)^2 = \sigma_i^\pm \sigma_i^\mp$. We thus write Eq.(3.60) as

$$\partial_t \rho = -i[H_0 + H_{\text{int}}, \rho] + \sum_{i=1}^3 \sum_{\mu=1}^4 \gamma_i^\mu \left(2L_i^\mu \rho L_i^{\mu\dagger} - \{L_i^{\mu\dagger} L_i^\mu, \rho\} \right), \tag{3.65}$$

where $\gamma_i^1 = \gamma_i^2 = p_i \bar{r}_i / 2$, $\gamma_i^3 = \gamma_i^4 = p_i r_i / 2$, $L_i^1 = \sigma_i^+$, $L_i^2 = \sigma_i^+ \sigma_i^-$, $L_i^3 = \sigma_i^-$ and $L_i^4 = \sigma_i^- \sigma_i^+$. This equation does not have detailed balance, or equivalently, has a NESS. In the following we obtain a repeated interaction in which each bath alternates two different couplings with its corresponding qubit. We will find that the work done due to turning on and off the interaction between the baths and the system in the repeated interaction are in the continuous limit given by the powers

$$\dot{W}_i = -p_i \text{Tr}_S[H_{\text{int}} \rho_S], \tag{3.66}$$

while the heat fluxes are

$$\dot{Q}_i = \frac{1}{2} E_i p_i (\text{Tr}_S[\sigma_i^z \rho_S] - (1 - 2r_i)). \tag{3.67}$$

To construct a bath and coupling so that Eq.(3.65) is obtained from a repeated interaction we propose the following *ansatz*, where two different couplings between the bath r and the qubit i alternate. These are given by

$$V_r^Q = J_r (\sigma_r^x \sigma_i^x + \sigma_r^y \sigma_i^y + Q_r (\sigma_r^z - M_r) \sigma_i^z), \quad V_r^P = J_r (\sigma_r^x \sigma_i^x + \sigma_r^y \sigma_i^y + P_r (\sigma_r^z - M_r) \sigma_i^z), \tag{3.68}$$

where $r = \{C, R, H\}$ indicates the bath and are associated with $i = \{1, 2, 3\}$ representing the three qubits. The coefficients Q_r and P_r are unknown and for the moment are part of the *ansatz*. The other coefficient is $M_r = \text{Tr}_r[\sigma_r^z \rho_r^n(0)]$ (see below $\rho_r^n(0)$). As in Section 1.2 we assume that the bath r has Hamiltonian $H_r = \bigoplus_n H_r^n$ where $H_r^n = -(E_r/2) \sigma_r^z$. The system and baths are initially uncorrelated, $\rho(0) = \rho_S(0) \bigotimes_r \rho_r(0)$, where $\rho_r(0) = \bigotimes_n \rho_r^n(0) = \bigotimes_n \omega_{\beta_r}(H_r^n)$. The interaction between the system and baths is divided into $2N$ steps of time τ from $t = 0$ to $t = T = 2N\tau$. In even time steps the system-bath coupling is $V^Q = \sum_r V_r^Q$ and in odd time steps is $V^P = \sum_r V_r^P$. The evolution after the first two time steps reads

$$\rho(\tau) = U_1^Q (\rho_S(0) \otimes \rho_1) U_1^{Q\dagger} \otimes \rho_2 \otimes \rho_3 \otimes \dots \tag{3.69}$$

$$\rho_{\text{tot}}(2\tau) = \mathcal{U}_2^P (U_1^Q (\rho_S(0) \otimes \rho_1) U_1^{Q\dagger} \otimes \rho_2) \mathcal{U}_2^{P\dagger} \otimes \rho_3 \otimes \dots \tag{3.70}$$

where $U_1^Q = e^{-i\tau(H_S + \sum_r H_r^1 + V_r^Q)}$ and $U_2^P = e^{-i\tau(H_S + \sum_r H_r^2 + V_r^P)} e^{-it \sum_r H_r^1}$. Tracing out the baths the recurrence obtained is

$$\rho_S((2n-1)\tau) = \text{Tr}_{(2n-1)} \left(U_{(2n-1)}^Q(\tau) (\rho_S((2n-2)\tau) \otimes \rho_{(2n-1)}) U_{(2n-1)}^{Q\dagger}(\tau) \right) \tag{3.71}$$

$$\rho_S(2n\tau) = \text{Tr}_{2n} \left(U_{2n}^P(\rho_S((2n-1)\tau) \otimes \rho_{2n}) U_{2n}^{P\dagger} \right). \quad (3.72)$$

Since ρ_n and H_α^n are the same for every n , we can drop the label on ρ_n and $U_n^{Q,P}$, writing just

$$\rho_S((2n-1)\tau) = \text{Tr}_E \left(U^Q(\rho_S((2n-2)\tau) \otimes \rho_E) U^{Q\dagger} \right) \quad (3.73)$$

$$\rho_S(2n\tau) = \text{Tr}_E \left(U^P(\rho_S((2n-1)\tau) \otimes \rho_E) U^{P\dagger} \right). \quad (3.74)$$

Now we expand U^R , where $R = \{Q, P\}$ for small τ up to order $\tau^{3/2}$. Scaling the couplings as $V_r^R = v_r^R/\sqrt{\tau}$ we obtain

$$U^R(\tau) = I - iv^R \tau^{\frac{1}{2}} - \left(iH_{SE} + \frac{(v^R)^2}{2} \right) \tau - \frac{1}{2} \{H_0, v^R\} \tau^{\frac{3}{2}} + \mathcal{O}(\tau^2), \quad (3.75)$$

where $H_{SE} = H_S + \sum_r H_r$ and $v^R = \sum_r v_r^R$. Thus we have

$$\begin{aligned} \rho_S(2n\tau) - \rho_S((2n-1)\tau) &= \text{Tr}_E \left(U^P \rho_S((2n-1)\tau) \otimes \rho_E U^{P\dagger} - \rho_S((2n-1)\tau) \otimes \rho_E \right) \\ &= -i\tau [H_S, \rho_S((2n-1)\tau)] + \tau \text{Tr}_E \left(v^P \rho_S((2n-1)\tau) \otimes \rho_E v^P \right) \\ &\quad - \frac{\tau}{2} \text{Tr}_E \left\{ (v^P)^2, \rho_S((2n-1)\tau) \otimes \rho_E \right\} + \mathcal{O}(\tau^{3/2}), \end{aligned} \quad (3.76)$$

and also

$$\begin{aligned} \rho_S((2n-1)\tau) - \rho_S((2n-2)\tau) &= \text{Tr}_E \left(U^Q \rho_S((2n-2)\tau) \otimes \rho_E U^{Q\dagger} - \rho_S((2n-2)\tau) \otimes \rho_E \right) \\ &= -i\tau [H_S, \rho_S((2n-2)\tau)] + \tau \text{Tr}_E \left(v^Q \rho_S((2n-2)\tau) \otimes \rho_E v^Q \right) \\ &\quad - \frac{\tau}{2} \text{Tr}_E \left\{ (v^Q)^2, \rho_S((2n-2)\tau) \otimes \rho_E \right\} + \mathcal{O}(\tau^{3/2}), \end{aligned} \quad (3.77)$$

where we have used that $\text{Tr}_E[v^R \rho_S \otimes \rho_E] = 0$ (for which we need that $M_r = \text{Tr}_E[\sigma_r^z \omega_{\beta_r}(H_r)]$) and $\text{Tr}_E[H_r, \rho_S \otimes \rho_E] = 0$. Summing Eqs.(3.76) and (3.77), dividing by 2τ and taking the limit $\tau \rightarrow 0$ and $n \rightarrow \infty$ such that $2n\tau = t$ is finite we obtain

$$\dot{\rho}_S = -i[H_S, \rho_S] + \frac{1}{2} \mathcal{D}^Q(\rho_S) + \frac{1}{2} \mathcal{D}^P(\rho_S), \quad (3.78)$$

with $\mathcal{D}^R(\rho_S) = \text{Tr}_E [v^R(\rho_S \otimes \rho_E)v^R] - \frac{1}{2} \text{Tr}_E \left\{ (v^R)^2, \rho_S \otimes \rho_E \right\}$. Since $v^R = \sum_r v_r^R$ and $\text{Tr}_r(v_r^R \omega_r) = 0$, this equation can be split as

$$\dot{\rho}_S = -i\tau [H_S, \rho_S] + \frac{1}{2} \sum_r \mathcal{D}_r^Q(\rho_S) + \frac{1}{2} \sum_r \mathcal{D}_r^P(\rho_S), \quad (3.79)$$

with $\mathcal{D}_r^R(\rho_S) = \text{Tr}_r [v_r^R(\rho_S \otimes \rho_E)v_r^R] - \frac{1}{2} \text{Tr}_r \left\{ (v_r^R)^2, \rho_S \otimes \rho_E \right\}$.

Using $J_r = \sqrt{\lambda_r/\tau}$ and replacing the couplings, Eq.(3.68), into Eq.(3.79) we obtain for the dissipator $\frac{1}{2}(\mathcal{D}^Q(\rho_S) + \mathcal{D}^P(\rho_S))$ the following (we write ρ_S as ρ for the moment to simplify

the notation):

$$\begin{aligned} & \frac{1}{2} \sum_i \lambda_r \left[2(1 + M_r) \left(\sigma_i^+ \rho \sigma_i^- - \frac{1}{2} \{ \sigma_i^- \sigma_i^+, \rho \} \right) + 2(1 - M_r) \left(\sigma_i^- \rho \sigma_i^+ - \frac{1}{2} \{ \sigma_i^+ \sigma_i^-, \rho \} \right) \right. \\ & \quad \left. + 4Q_i^2(1 - M_r^2) \left(\sigma_i^+ \sigma_i^- \rho \sigma_i^+ \sigma_i^- - \frac{1}{2} \{ \sigma_i^+ \sigma_i^-, \rho \} \right) \right] \\ & + \frac{1}{2} \sum_i \lambda_i \left[2(1 + M_i) \left(\sigma_i^+ \rho \sigma_i^- - \frac{1}{2} \{ \sigma_i^- \sigma_i^+, \rho \} \right) + 2(1 - M_r) \left(\sigma_i^- \rho \sigma_i^+ - \frac{1}{2} \{ \sigma_i^+ \sigma_i^-, \rho \} \right) \right. \\ & \quad \left. + 4P_i^2(1 - M_r^2) \left(\sigma_i^+ \sigma_i^- \rho \sigma_i^+ \sigma_i^- - \frac{1}{2} \{ \sigma_i^+ \sigma_i^-, \rho \} \right) \right] \end{aligned}$$

(Note that r and i come in pairs $\{r, i\} = \{\{C, 1\}, \{R, 2\}, \{H, 3\}\}$.) Choosing $Q_i^2 = (1 - M_r)^{-1}$ and $P_i^2 = (1 + M_r)^{-1}$ we obtain

$$\begin{aligned} & \sum_i \lambda_i \left[(1 + M_r) \left(2\sigma_i^+ \rho \sigma_i^- - \{ \sigma_i^- \sigma_i^+, \rho \} \right) + (1 - M_r) \left(2\sigma_i^- \rho \sigma_i^+ - \{ \sigma_i^+ \sigma_i^-, \rho \} \right) \right. \\ & \quad \left. + (1 + M_r) \left(2\sigma_i^+ \sigma_i^- \rho \sigma_i^+ \sigma_i^- - \{ \sigma_i^+ \sigma_i^-, \rho \} \right) + (1 - M_r) \left(2\sigma_i^- \sigma_i^+ \rho \sigma_i^- \sigma_i^+ - \{ \sigma_i^- \sigma_i^+, \rho \} \right) \right]. \end{aligned}$$

Note that $(1 \pm M_r) = 1 + \text{Tr}_r[\sigma_r^z \rho_r] = 2 \text{Tr}_r[\sigma_r^\pm \sigma_r^\mp \rho_r]$. If we re-scale the energy spectrum of the bath such that $H_r = E_i |1\rangle_r \langle 1|_r$ with the same energy for the excited state as the corresponding refrigerator qubit i , we have that $(1 + M_r) = 2\bar{r}_i$ and $(1 - M_r) = 2r_i$ (recall that $r_i = \langle 0|_i \omega_{\beta_i}(H_i) |0\rangle_i$ and $\bar{r}_i = \langle 1|_i \omega_{\beta_i}(H_i) |1\rangle_i$). Additionally we choose $\lambda_r = p_i/4$ and we recover the Lindblad form for the three qubit refrigerator, Eq.(3.65),

$$\begin{aligned} \dot{\rho}_S &= -i[H_S, \rho_S] \\ & + \sum_i \frac{1}{2} p_i \bar{r}_i \left(2\sigma_i^+ \rho_S \sigma_i^- - \{ \sigma_i^- \sigma_i^+, \rho_S \} + 2\sigma_i^+ \sigma_i^- \rho_S \sigma_i^+ \sigma_i^- - \{ \sigma_i^+ \sigma_i^-, \rho_S \} \right) \\ & + \sum_i \frac{1}{2} p_i r_i \left(2\sigma_i^- \rho_S \sigma_i^+ - \{ \sigma_i^+ \sigma_i^-, \rho_S \} + 2\sigma_i^- \sigma_i^+ \rho_S \sigma_i^- \sigma_i^+ - \{ \sigma_i^- \sigma_i^+, \rho_S \} \right). \end{aligned} \quad (3.80)$$

In same manner that we obtained in Section 1.2 the expressions for the heat and work, here we have

$$\Delta Q_{r,2n\tau}^P = \text{Tr}_{2n}[H_r(\rho_{2n} - \rho'_{2n})], \quad (3.81)$$

$$\Delta Q_{r,(2n+1)\tau}^Q = \text{Tr}_{2n+1}[H_r(\rho_{2n+1} - \rho'_{2n+1})], \quad (3.82)$$

where $\rho'_m = \text{Tr}_S[U_m \rho_S((m-1)\tau) \otimes \rho_E U_m^\dagger]$ is the density matrix of the m -copy of the bath after the interaction, and

$$\Delta W_{2n\tau} = \text{Tr}[\rho(2n\tau)(V_{2n+1} - V_{2n})] = -\text{Tr}[U_{2n} \rho_S((2n-1)\tau) \otimes \rho_E U_{2n}^\dagger V_{2n}], \quad (3.83)$$

$$\Delta W_{(2n+1)\tau} = \text{Tr}[\rho(2n\tau)(V_{2n+2} - V_{2n+1})] = -\text{Tr}[U_{2n+1} \rho_S(2n\tau) \otimes \rho_E U_{2n+1}^\dagger V_{2n+1}], \quad (3.84)$$

Doing the scaling $V = v/\sqrt{\tau}$, expanding these expressions up to order τ , dividing by 2τ and taking the limits we obtain the heat fluxes

$$\dot{Q}_r \equiv \frac{1}{2}\dot{Q}_r^P + \frac{1}{2}\dot{Q}_r^Q = -\frac{1}{2}D_r^P(H_r) - \frac{1}{2}D_r^Q(H_r) \quad (3.85)$$

and the powers

$$\dot{W}_r \equiv \frac{1}{2}\dot{W}_r^P + \frac{1}{2}\dot{W}_r^Q = \frac{1}{2}D_r^P(H_S + H_r) + \frac{1}{2}D_r^Q(H_S + H_r), \quad (3.86)$$

where $D_r^R(A) = \text{Tr}[(v_r^R A v_r^R - \frac{1}{2}\{(v_r^R)^2, A\})\rho_s(t) \otimes \omega_{\beta_r}(H_r)]$. For our particular system, these expressions are Eqs.(3.67) and (3.66), respectively.

It can be shown with thermodynamical arguments that the efficiency of a refrigerator composed of three baths where only heat fluxes are interchanged like the one in [48, 31] is given by $\eta = \dot{Q}_C/\dot{Q}_H$. In our analysis, this expression changes to $\eta = \dot{Q}_C/(\dot{Q}_H + \sum_i \dot{W}_i)$. We thus argue that a boundary driven Lindblad equation of the form Eq.(3.65) can be microscopically derived from the repeated interaction scheme, but it will not be an autonomous refrigerator as conceived initially since it needs external work $\sum_i \dot{W}_i$.

Conclusions

We have studied the stochastic thermodynamics of CPTP quantum maps discussing in particular the properties of maps with equilibrium. Thermal maps are a very important class of maps with equilibrium because they represent the passive effect of a heat bath on a system, while non-thermal maps with equilibrium require the active intervention of an agent, manifested by the work required to perform the process represented by \mathcal{E} even when the system Hamiltonian is not driven. We have shown that for maps with equilibrium the thermodynamic quantities can be written in local form, this means, in terms of system's operators. This is a great simplification since the experimenter usually does not have access to the state of the bath after the interaction, this might be because the bath has many particles and/or (like in the repeated interaction) there are many baths interacting with the system.

Non-thermal maps with equilibrium are, in a sense, in between thermal maps and maps with non-equilibrium steady states. They share thermal maps' simplicity of relaxing to the equilibrium state, while at the same time allow us to study energy exchanges between the system, the bath and the experimenter in a non-trivial case. The result we have illustrated here might not be restricted to quantum systems, but in quantum systems the manipulation of the interaction with the environment is much better controlled and thus the possibility of transforming the state of a system using *active* interactions $V(t)$ with the environment as illustrated with the XX spin 1/2 chain is already in the tool box of the experimentalist [50]. We believe that an implementation of the XX chain with trapped ions and the interaction with probes by its boundary is possible and that it can be a candidate to investigate further aspects of quantum thermodynamics. Recently, the Landauer principle was experimentally verified in nuclear spins of molecules on a NMR set-up [51]. In this experiment, quantum state tomography is used to determine the system's entropy change, and for the bath, an auxiliary system (an ancilla qubit) is used to reconstruct the heat exchange probability distribution of the process. On previous NMR experiments (see references in [51]) it was also possible to determine work distributions. This means that this set-up could be used to verify if the local thermodynamics quantities when the CPTP map has equilibrium are correct.

Stochastic thermodynamics for classical systems with Hamiltonian or stochastic dynamics (Langevin or discrete master equation) is usually formulated for systems with the properties we associate to thermal operations: in the absence of driving the system thermalizes to the corresponding Gibbs state and the stochastic work is zero in non-driven systems. For instance, in classical stochastic thermodynamics, and for thermal maps too, a system in equilibrium presents no entropy production fluctuation and this implies no work fluctuations either. In the quantum case one can consider these fluctuations simultaneously if the equilibrium state

commutes with the Hamiltonian of the system. We have seen that in the XX spin 1/2 chain we have studied, where the dynamics is controlled by a non-thermal map with equilibrium, and where the equilibrium state commutes with the Hamiltonian, it is possible to have a fluctuating work and no entropy production fluctuations.

On the other hand, open systems, in contact with a single heat bath, whose dynamics is represented by a map without equilibrium (its invariant state is a non-equilibrium state), presents a complexity similar to the one of open systems passively coupled to two heat baths at different temperatures. Nevertheless a few properties for this case were also studied like the statistics of work for systems starting in the Gibbs $\omega_\beta(H_S)$ state, Eq.(2.23).

We have generalized the condition of equilibrium in Lindblad master equations through the generalization of the detailed balance condition which has allowed us to relate this condition with the equilibrium of a CPTP map when it is iterated. We argued that when a Lindblad equation has detailed balance it is straightforward to obtain a repeated interaction that generates it, thus heat, work and entropy production can be defined in a consistent way in local form (in terms of operators of the system) for any coupling strength. We emphasize that this might be used as a tool for designing quantum thermal machines with boundary driven Lindblad equations dynamics. As a final remark, we would like to point out that this simplification in the thermodynamic quantities in the presence of a equilibrium has been derived when there is only one temperature for the possibly many baths. When there are different temperatures, one might only be able to write the sum of the heats and the entropy production in local form, but not the work, thus further exploration is required.

Appendix A

Proof of Eq.(2.20)

Eq.(2.20) is an equality between operators in the system Hilbert space \mathcal{H}_S that we can write as

$$\langle \tilde{i} | \tilde{U} | \tilde{j} \rangle = \Theta_S \langle j | U | i \rangle^\dagger \Theta_S^\dagger$$

where $\tilde{U} = \Theta U^\dagger \Theta^\dagger$ and $|\tilde{i}\rangle = \Theta_B |i\rangle$. We prove it by showing that the matrix elements in an arbitrary basis are the same. Consider the operator at the left hand side and evaluate its matrix elements with states $|\tilde{a}\rangle = \Theta_S |a\rangle$ and $|\tilde{b}\rangle = \Theta_S |b\rangle$, i.e.,

$$\begin{aligned} \left(|\tilde{a}\rangle, \langle \tilde{i} | \tilde{U} | \tilde{j} \rangle | \tilde{b} \rangle \right)_{\mathcal{H}_S} &= \left(|\tilde{a}\tilde{i}\rangle, \tilde{U} |\tilde{b}\tilde{j}\rangle \right)_{\mathcal{H}_{\text{tot}}} = \left(\Theta |ai\rangle, \Theta U^\dagger |bj\rangle \right)_{\mathcal{H}_{\text{tot}}} \\ &= \left(U^\dagger |bj\rangle, |ai\rangle \right)_{\mathcal{H}_{\text{tot}}} = \langle bj | U | ai \rangle. \end{aligned} \quad (\text{A.1})$$

Let us now evaluate the same element for the operator in the right hand side

$$\begin{aligned} \left(|\tilde{a}\rangle, \Theta_S \langle j | U | i \rangle^\dagger \Theta_S^\dagger | \tilde{b} \rangle \right)_{\mathcal{H}_S} &= \left(\Theta_S |a\rangle, \Theta_S \langle j | U | i \rangle^\dagger |b\rangle \right)_{\mathcal{H}_S} = \left(\langle j | U | i \rangle^\dagger |b\rangle, |a\rangle \right)_{\mathcal{H}_S} \\ &= \left(|b\rangle, \langle j | U | i \rangle |a\rangle \right)_{\mathcal{H}_S} = \langle bj | U | ai \rangle \end{aligned} \quad (\text{A.2})$$

and therefore we have the equality. Note that we have used the property $(\Theta\phi, \Theta\psi) = (\psi, \phi)$ that the anti-unitary operators Θ and Θ_S satisfy in the corresponding Hilbert space.

Appendix B

$p(w) = \tilde{p}(w)$ if the Hamiltonian H_{tot} is invariant under time reversal.

For the spin systems we consider in our analysis and the time reversal operator Θ defined in Section 2.6, we have the equality $\tilde{U} = U$, which equivalently means that the Hamiltonian H_{tot} is invariant under time reversal. We will now show that this implies that the work distribution of the forward process equals the work distribution of the reversed process, $p(w) = \tilde{p}(w)$. For every trajectory $\gamma = \{n, k, m\}$ in the forward process there is a associated backward trajectory $\tilde{\gamma} = \{\tilde{m}, \tilde{k}, \tilde{n}\}$, but now we will compare γ with another trajectory belonging to the backward trajectories, that is $\tilde{\gamma}' = \{\tilde{n}, -\tilde{k}, \tilde{m}\}$ where if $k = ij$ is associated with the Kraus operator $M_{k=ij}$, then $-\tilde{k}$ corresponds to the operator \tilde{M}_{ij} (see Eq.(2.19)). Note that if we measure the system energy at the beginning and at the end, $|a_n\rangle$ and $|b_m\rangle$ correspond to energy eigenstates. Due to the fact that the Hamiltonian is invariant under time reversal, we have that $\Theta_S |a_n\rangle = |a_n\rangle$ and $\Theta_S |b_m\rangle = |b_m\rangle$ (the same is true for the energy eigenstates of the bath, $\Theta_B |i\rangle = |i\rangle$ and $\Theta_B |j\rangle = |j\rangle$), thus according to Eq.(2.19) we get $\tilde{M}_{ij} = M_{ij}$. These trajectories are:

$$|n\rangle \xrightarrow{k} |m\rangle, \quad p(\gamma) = p_i(n) |\langle b_m | M_{ij} | a_n \rangle|^2, \quad \beta w_\gamma = \ln \frac{p_i(n)}{p_i(m)} - \beta(\varepsilon_i - \varepsilon_j) \quad (\text{B.1})$$

$$|\tilde{n}\rangle \xrightarrow{-\tilde{k}} |\tilde{m}\rangle, \quad \tilde{p}(\tilde{\gamma}') = p_i(n) |\langle \tilde{b}_m | \tilde{M}_{ij} | \tilde{a}_n \rangle|^2, \quad \beta w_{\tilde{\gamma}'} = \ln \frac{p_i(n)}{p_i(m)} - \beta(\varepsilon_i - \varepsilon_j). \quad (\text{B.2})$$

Those two probabilities are the same, $p(\gamma) = \tilde{p}(\tilde{\gamma}')$ and $w_\gamma = w_{\tilde{\gamma}'}$. We conclude that every trajectory in the forward process is also present in the backward process, so the work distribution is the same, $p(w) = \tilde{p}(w)$.

To derive an equivalent relation for the entropy production, $p(\Delta_i s) = \tilde{p}(\Delta_i s)$, we equivalently require that $\Theta |a_n\rangle = |a_n\rangle$ and $\Theta |b_m\rangle = |b_m\rangle$, however, now these states are the initial density matrix and final density matrix eigenstates. We thus need time reversal invariant initial and final density matrices, i.e., $\Theta \rho \Theta^\dagger = \rho$ and $\Theta \rho' \Theta^\dagger = \rho'$. In the stationary state of the XX spin chain this is fulfilled, since $\rho_{XX} = e^{-\beta H_0} / Z_0$ is invariant under time reversal with Θ defined as in Section 2.6. However, for the XY stationary state, this is not true, since $\rho_{XY} \neq \Theta \rho_{XY} \Theta^\dagger$.

The previous analysis can be readily generalized to a concatenation of maps and the same results hold.

Appendix C

Thermal maps do not contribute to work fluctuations

To demonstrate that in the thermodynamic cycle of Section 2.6.1 the work probability distribution is determined only by the driving, $p_{\text{cycle}}(w) = p_{\text{drive}}(w)$, we assume that there is just one thermalization map. The generalization to many thermalization maps, though, is straight forward.

The work distribution probability is

$$\begin{aligned} p(w) &= \sum_{\gamma} p(\gamma) \delta(\epsilon_m - \epsilon_n - q_{\gamma} - w) \\ &= \sum_{\gamma} p_i(n) p_{i_1} p_{i_2} |\langle \epsilon_m, \epsilon_{j_1}, \epsilon_{j_2} | U_2 U_1 | \epsilon_n, \epsilon_{i_1}, \epsilon_{i_2} \rangle|^2 \delta(\epsilon_m - \epsilon_n - q_{\gamma} - w), \end{aligned} \quad (\text{C.1})$$

where U_1 is responsible for the driving and U_2 for the thermalization. The probabilities are $p_i(n) = e^{-\beta \epsilon_n} / Z_S$ and $p_{i_k} = e^{-\beta \epsilon_{i_k}} / Z_b$, and $\delta(\cdot)$ is a Kronecker-Delta. Expanding the transition probability and including two identities in the system Hilbert space \mathcal{H}_S we get

$$p(w) = \sum_{\gamma, \alpha, \beta} p_i(n) p_{i_1} p_{i_2} |\langle \epsilon_m, \epsilon_{j_2} | U_2 | \epsilon_{\alpha}, \epsilon_{i_2} \rangle \langle \epsilon_{\alpha}, \epsilon_{j_1} | U_1 | \epsilon_n, \epsilon_{i_1} \rangle \langle \epsilon_n, \epsilon_{i_1} | U_1^{\dagger} | \epsilon_{\beta}, \epsilon_{j_1} \rangle \langle \epsilon_{\beta}, \epsilon_{i_2} | U_2^{\dagger} | \epsilon_m, \epsilon_{j_2} \rangle \delta(\epsilon_m - \epsilon_n - q_{\gamma} - w)|^2$$

Since U_2 is thermal, $\epsilon_m + \epsilon_{j_2} = \epsilon_{\alpha} + \epsilon_{i_2} = \epsilon_{\beta} + \epsilon_{i_2}$, thus, since the system Hamiltonian is non-degenerate, $\alpha = \beta$. Additionally, we can replace $\epsilon_m = \epsilon_{\alpha} + \epsilon_{i_2} - \epsilon_{j_2}$ in the delta, obtaining

$$p(w) = \sum_{\gamma, \alpha} p_i(n) p_{i_1} p_{i_2} |\langle \epsilon_{\alpha}, \epsilon_{j_1} | U_1 | \epsilon_n, \epsilon_{i_1} \rangle|^2 |\langle \epsilon_m, \epsilon_{j_2} | U_2 | \epsilon_{\alpha}, \epsilon_{i_2} \rangle|^2 \delta(\epsilon_{\alpha} - \epsilon_n + \epsilon_{j_1} - \epsilon_{i_1} - w). \quad (\text{C.2})$$

Summing over m and j_2 the second transition probability becomes a trace, which is equal to one. Finally we arrive to

$$p(w) = \sum_{\alpha, j_1, n, i_1} p_i(n) p_{i_1} |\langle \epsilon_{\alpha}, \epsilon_{j_1} | U_1 | \epsilon_n, \epsilon_{i_1} \rangle|^2 \delta(\epsilon_{\alpha} - \epsilon_n + \epsilon_{j_1} - \epsilon_{i_1} - w). \quad (\text{C.3})$$

Note that this quantity is exactly the work distribution probability of the driving alone, thus $p_{\text{cycle}}(w) = p_{\text{drive}}(w)$. We remark that this implies also that $p_{\text{cycle}}(w) = \tilde{p}_{\text{cycle}}(w)$ despite of

the fact that the protocol is not symmetric (because in the backward process the relaxation map acts first).

Bibliography

- [1] Christopher Jarzynski. Equilibrium free-energy differences from nonequilibrium measurements: A master-equation approach. *Phys. Rev. E*, 56:5018–5035, Nov 1997.
- [2] Christopher Jarzynski. Nonequilibrium equality for free energy differences. *Phys. Rev. Lett.*, 78:2690–2693, Apr 1997.
- [3] Gavin E. Crooks. Nonequilibrium measurements of free energy differences for microscopically reversible markovian systems. *Journal of Statistical Physics*, 90(5):1481–1487, 1998.
- [4] Gavin E. Crooks. Entropy production fluctuation theorem and the nonequilibrium work relation for free energy differences. *Phys. Rev. E*, 60:2721–2726, Sep 1999.
- [5] Jan Liphardt, Sophie Dumont, Steven B. Smith, Ignacio Tinoco, and Carlos Bustamante. Equilibrium information from nonequilibrium measurements in an experimental test of jarzynski’s equality. *Science*, 296(5574):1832–1835, 2002.
- [6] Felix Ritort. Single-molecule experiments in biological physics: methods and applications. *Journal of Physics: Condensed Matter*, 18(32):R531, 2006.
- [7] Valentin. Blickle, Thomas. Speck, Laurent Helden, Udo Seifert, and Clemens Bechinger. Thermodynamics of a colloidal particle in a time-dependent nonharmonic potential. *Phys. Rev. Lett.*, 96:070603, Feb 2006.
- [8] Hal Tasaki. Jarzynski Relations for Quantum Systems and Some Applications. *eprint arXiv:cond-mat/0009244*, September 2000.
- [9] Jorge Kurchan. A Quantum Fluctuation Theorem. *eprint arXiv:cond-mat/0007360*, July 2000.
- [10] Gavin E. Crooks. On the jarzynski relation for dissipative quantum dynamics. *J. Stat. Mech. Theor. Exp.*, 2008(10):P10023, 2008.
- [11] Tiago B. Batalhão, Alexandre M. Souza, Laura Mazzola, Ruben Auccaise, Roberto S. Sarthour, Ivan S. Oliveira, John Goold, Gabriele De Chiara, Mauro Paternostro, and Roberto M. Serra. Experimental reconstruction of work distribution and study of fluctuation relations in a closed quantum system. *Phys. Rev. Lett.*, 113:140601, Oct 2014.

- [12] Shuoming An, Jing-Ning Zhang, Mark Um, Lv Dingshun, Yao Lu, Junhua Zhang, Zhang-Qi Yin, H. T. Quan, and Kihwan Kim. Experimental test of the quantum jarzynski equality with a trapped-ion system. *Nat. Phys.*, 11:193–199, 2015.
- [13] Rrobert Alicki. The quantum open system as a model of the heat engine. *Journal of Physics A: Mathematical and General*, 12(5):L103, 1979.
- [14] Herbert Spohn and Joel L. Lebowitz. *Irreversible Thermodynamics for Quantum Systems Weakly Coupled to Thermal Reservoirs*, pages 109–142. John Wiley & Sons, Inc., 2007.
- [15] Heinz-Peter Breuer and Francesco Petruccione. *The Theory of Open Quantum Systems*. OUP Oxford, 2007.
- [16] Felipe Barra. The thermodynamic cost of driving quantum systems by their boundaries. *Scientific Reports*, 5:14873, Oct 2015. Article.
- [17] Michael A. Nielsen and Isaac L. Chuang. *Quantum Computation and Quantum Information: 10th Anniversary Edition*. Cambridge University Press, New York, NY, USA, 10th edition, 2011.
- [18] Massimiliano Esposito, Katja Lindenberg, and Christian Van den Broeck. Entropy production as correlation between system and reservoir. *New Journal of Physics*, 12(1):013013, 2010.
- [19] Udo Seifert. First and second law of thermodynamics at strong coupling. *Phys. Rev. Lett.*, 116:020601, Jan 2016.
- [20] Thomas G. Philbin and Janet Anders. Thermal energies of classical and quantum damped oscillators coupled to reservoirs. *Journal of Physics A: Mathematical and Theoretical*, 49(21):215303, 2016.
- [21] Christopher Jarzynski. Stochastic and macroscopic thermodynamics of strongly coupled systems. *Phys. Rev. X*, 7:011008, Jan 2017.
- [22] Jordan M. Horowitz and Juan M. R. Parrondo. Entropy production along nonequilibrium quantum jump trajectories. *New Journal of Physics*, 15(8):085028, 2013.
- [23] David Reeb and Michael M Wolf. An improved landauer principle with finite-size corrections. *New Journal of Physics*, 16(10):103011, 2014.
- [24] Gonzalo Manzano, Jordan M. Horowitz, and Juan M. R. Parrondo. Nonequilibrium potential and fluctuation theorems for quantum maps. *Phys. Rev. E*, 92:032129, Sep 2015.
- [25] Massimiliano Esposito, Upendra Harbola, and Shaul Mukamel. Nonequilibrium fluctuations, fluctuation theorems, and counting statistics in quantum systems. *Rev. Mod. Phys.*, 81:1665–1702, Dec 2009.
- [26] Philippe Faist, Jonathan Oppenheim, and Renato Renner. Gibbs-preserving maps

- outperform thermal operations in the quantum regime. *New Journal of Physics*, 17(4):043003, 2015.
- [27] Philipp Strasberg, Gernot Schaller, Tobias Brandes, and Massimiliano Esposito. Quantum and information thermodynamics: A unifying framework based on repeated interactions. *Phys. Rev. X*, 7:021003, Apr 2017.
- [28] Sai Vinjanampathy and Janet Anders. Quantum thermodynamics. *Contemporary Physics*, 57(4):545–579, 2016.
- [29] Sebastian Deffner and Eric Lutz. Nonequilibrium entropy production for open quantum systems. *Phys. Rev. Lett.*, 107:140404, Sep 2011.
- [30] Bojan Žunkovič and Tomaž Prosen. Explicit solution of the lindblad equation for nearly isotropic boundary driven xy spin 1/2 chain. *Journal of Statistical Mechanics: Theory and Experiment*, 2010(08):P08016, 2010.
- [31] Paul Skrzypczyk, Nicolas Brunner, Noah Linden, and Sandu Popescu. The smallest refrigerators can reach maximal efficiency. *Journal of Physics A: Mathematical and Theoretical*, 44(49):492002, 2011.
- [32] Tomaž Prosen. Matrix product solutions of boundary driven quantum chains. *Journal of Physics A: Mathematical and Theoretical*, 48(37):373001, 2015.
- [33] Vladislav Popkov and Gunter M. Schütz. Solution of the lindblad equation for spin helix states. *Phys. Rev. E*, 95:042128, Apr 2017.
- [34] Stéphane Attal and Yan Pautrat. From repeated to continuous quantum interactions. *Annales Henri Poincaré*, 7(1):59–104, 2006.
- [35] Dragi Karevski and Thierry Platini. Quantum nonequilibrium steady states induced by repeated interactions. *Phys. Rev. Lett.*, 102:207207, May 2009.
- [36] Udo Seifert. Stochastic thermodynamics: principles and perspectives. *The European Physical Journal B*, 64(3):423–431, 2008.
- [37] Christian Van den Broeck and Massimiliano Esposito. Ensemble and trajectory thermodynamics: A brief introduction. *Physica A: Statistical Mechanics and its Applications*, 418:6 – 16, 2015.
- [38] Sania Jevtic, Terry Rudolph, David Jennings, Yuji Hirono, Shojun Nakayama, and Mio Murao. Exchange fluctuation theorem for correlated quantum systems. *Phys. Rev. E*, 92:042113, Oct 2015.
- [39] Matteo Lostaglio, Kamil Korzekwa, David Jennings, and Terry Rudolph. Quantum coherence, time-translation symmetry, and thermodynamics. *Phys. Rev. X*, 5:021001, Apr 2015.
- [40] Matteo Lostaglio, David Jennings, and Terry Rudolph. Description of quantum co-

herence in thermodynamic processes requires constraints beyond free energy. *Nature Communications*, 6:6383, Mar 2015. Article.

- [41] Fritz Haake. *Quantum Signatures of Chaos*. Springer-Verlag Berlin Heidelberg, 3rd edition, 2010.
- [42] David Andrieux and Pierre Gaspard. Quantum work relations and response theory. *Phys. Rev. Lett.*, 100:230404, Jun 2008.
- [43] Michele Campisi, Peter Hänggi, and Peter Talkner. Colloquium. *Rev. Mod. Phys.*, 83:771–791, Jul 2011.
- [44] Dilip Kondepudi and Ilya Prigogine. *Modern Thermodynamics: From Heat Engines to Dissipative Structures*. John Wiley & Sons, Ltd, 2nd edition, 2014.
- [45] Robert Alicki. On the detailed balance condition for non-hamiltonian systems. *Reports on Mathematical Physics*, 10(2):249 – 258, 1976.
- [46] Andrzej Kossakowski, Alberto Frigerio, Vittorio Gorini, and Maurizio Verri. Quantum detailed balance and kms condition. *Comm. Math. Phys.*, 57(2):97–110, 1977.
- [47] Alberto Frigerio and Vittorio Gorini. Markov dilations and quantum detailed balance. *Comm. Math. Phys.*, 93(4):517–532, 1984.
- [48] Noah Linden, Sandu Popescu, and Paul Skrzypczyk. How small can thermal machines be? the smallest possible refrigerator. *Phys. Rev. Lett.*, 105:130401, Sep 2010.
- [49] Luis A. Correa, José P. Palao, Daniel Alonso, and Gerardo Adesso. Quantum-enhanced absorption refrigerators. *Scientific Reports*, 4:3949 EP –, Feb 2014. Article.
- [50] Philipp Schindler, Markus Müller, Daniel Nigg, Julio T. Barreiro, Esteban A. Martinez, Markus Hennrich, Thomas Monz, Sebastian Diehl, Peter Zoller, and Rainer Blatt. Quantum simulation of dynamical maps with trapped ions. *Nat Phys*, 9(6):361–367, Jun 2013. Article.
- [51] J. P. S. Peterson, R. S. Sarthour, A. M. Souza, I. S. Oliveira, J. Goold, K. Modi, D. O. Soares-Pinto, and L. C. Céleri. Experimental demonstration of information to energy conversion in a quantum system at the landauer limit. *Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences*, 472(2188), 2016.
- [52] Raam Uzdin, Amikam Levy, and Ronnie Kosloff. Equivalence of quantum heat machines, and quantum-thermodynamic signatures. *Phys. Rev. X*, 5:031044, Sep 2015.
- [53] Ronnie Kosloff and Amikam Levy. Quantum heat engines and refrigerators: Continuous devices. *Annual Review of Physical Chemistry*, 65(1):365–393, 2014. PMID: 24689798.
- [54] Kay Brandner and Udo Seifert. Periodic thermodynamics of open quantum systems. *Phys. Rev. E*, 93:062134, Jun 2016.

- [55] Udo Seifert. Entropy production along a stochastic trajectory and an integral fluctuation theorem. *Phys. Rev. Lett.*, 95:040602, Jul 2005.
- [56] Herbert Spohn. Entropy production for quantum dynamical semigroups. *Journal of Mathematical Physics*, 19(5):1227–1230, 1978.
- [57] Denis J. Evans, E. G. D. Cohen, and G. P. Morriss. Probability of second law violations in shearing steady states. *Phys. Rev. Lett.*, 71:3616–3616, Nov 1993.
- [58] Giovanni Gallavotti and Ezechiel G. D. Cohen. Dynamical ensembles in nonequilibrium statistical mechanics. *Phys. Rev. Lett.*, 74:2694–2697, Apr 1995.
- [59] Jorge Kurchan. Fluctuation theorem for stochastic dynamics. *Journal of Physics A: Mathematical and General*, 31(16):3719, 1998.
- [60] Joel L. Lebowitz and Herbert Spohn. A gallavotti–cohen-type symmetry in the large deviation functional for stochastic dynamics. *Journal of Statistical Physics*, 95(1):333–365, 1999.
- [61] David Andrieux, Pierre Gaspard, Takaaki Monnai, and Shuichi Tasaki. The fluctuation theorem for currents in open quantum systems. *New Journal of Physics*, 11(4):043014, 2009.
- [62] Delphine Collin, Felix Ritort, Christopher Jarzynski, Steven B. Smith, Ignacio Tinoco, and Carlos Bustamante. Verification of the crooks fluctuation theorem and recovery of rna folding free energies. *Nature*, 437(7056):231–234, Sep 2005.
- [63] Jordan M. Horowitz. Quantum-trajectory approach to the stochastic thermodynamics of a forced harmonic oscillator. *Phys. Rev. E*, 85:031110, Mar 2012.
- [64] Tomaž Prosen. Third quantization: a general method to solve master equations for quadratic open fermi systems. *New Journal of Physics*, 10(4):043026, 2008.
- [65] Tomaž Prosen. Spectral theorem for the lindblad equation for quadratic open fermionic systems. *Journal of Statistical Mechanics: Theory and Experiment*, 2010(07):P07020, 2010.