Non-equilibrium steady-states of memoryless quantum collision models

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We investigate the steady state properties arising from the open system dynamics described by a memoryless (Markovian) quantum collision model, corresponding to a master equation in the ultra-strong, singular coupling limit. By carefully assessing the work cost of switching on and off the system-environment interaction, we show that only a coupling Hamiltonian in the energy-preserving form drives the system to thermal equilibrium, while any other interaction leads to non-equilibrium states supported by steady-state currents. These currents provide a neat exemplification of the housekeeping work and heat. Furthermore, we show that the achievable non-equilibrium steady states can be non-passive and may also exhibit steady state coherence.

I. INTRODUCTION

Quantum thermodynamics [1–4] aims at describing energy exchanges, in the form of work and heat, between quantum systems, and allows for the study of the quantum source of irreversibility in non-equilibrium processes. A comprehensive understanding of such energetic exchanges is vital to extend our understanding of the laws of thermodynamics in the quantum regime, while also paving the way to exploit the peculiarities of quantum systems to realize efficient next generation quantum technologies.

While exquisite experimental control of many types of quantum systems and devices has been achieved to date, the unavoidable interaction with their surroundings has detrimental effects on their genuinely quantum properties, notably coherence and quantum correlations. The framework of open quantum systems allows us to account for these environmental effects through methods and models that provide a very accurate description of the system’s evolution [5, 6]. A particularly useful approach is given by the so-called quantum collision models, which constitute a very rich platform to simulate open quantum systems in a simple and yet reliable way [7–11]. Owing to their high flexibility, collision models have been utilized as a tool to study various physical phenomena, such as memory effects (or quantum non-Markovianity) [12–16], information erasure [17, 18], quantum thermodynamic processes [19–21], quantum synchronization [22], and the quantum-to-classical transition [23].

In this work, we exploit the versatility of collision models to fully characterize the steady-state thermodynamics for arbitrary system-environment interactions in the singular coupling limit, complementing the study of equilibration and thermalization via collision models [24–26]. In particular, we consider a system that interacts with an environment, consisting of an array of identical thermal constituents, in a memoryless (Markovian) collision model setting. We show that while the dynamics is fully described by a Gorini-Kossakowski-Sudarshan-Lindblad (GKSL) master equation, care must be taken in assessing the thermodynamics of the interaction process. More specifically, work, heat, and entropy production cannot generally be derived solely from the system’s degrees of freedom, but one needs to account for the interaction energy as well. Once this is satisfactorily taken into account and fully exploited, one is led to an elegant demonstration of the so-called housekeeping work and heat that maintain non-equilibrium steady states (NESS). Our results show that only an interaction in the energy-preserving form, or “thermal operations”, lead to thermalization with the environment, while all other interactions drive the system to a NESS.

The remainder of the paper is organized as follows. We start by introducing memoryless collision models and recall the derivation of their associated master equation in Sec. II. In Sec. III, we lay out the preliminaries for characterizing the thermodynamics of open systems and establish that, generally, the system is driven into a NESS supported by non-zero work and/or heat currents. We demonstrate our results for the case of a qubit collision model in Sec. IV, and, finally, we provide some concluding remarks in Sec. V.

II. MEMORYLESS COLLISION MODELS

Let us consider a system $S$, with Hamiltonian $\hat{H}_S$, coupled to an environment $E$ consisting of a series of identical non-interacting auxiliary units, each of them being described by the Hamiltonian $\hat{H}_A$, so that $\hat{H}_E = \sum_n \hat{H}_A^{(n)}$. The free evolution of the system, generated by $\hat{H}_S$, is punctuated by sequential interactions with the environmental units, each coupled to the system only once, for a time interval $\delta t$. This picture defines the so-called class of “repeated-interaction” or collision models [7–11]. Although more general situations can be envisaged [27, 28], in what follows we will restrict ourselves to regular-in-time system-environment couplings and assume that the time intervals between subsequent collisions, during which the system evolves unitarily, are negligible compared to $\delta t$. This means that, after having interacted with the $n$-th environmental unit for a time interval $\delta t$, the system immediately

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moves on to interact with the \((n+1)\)-th one.

A precise formulation of the above scheme is given by taking the system-environment interaction to be externally changed in time according to

\[
\hat{H}_{SE}(t) = \sum_n \Theta(t-n\delta t) \Theta((n+1)\delta t - t) \hat{H}_{SA},
\]

where \(\Theta(\cdot)\) denotes the Heaviside step function. A given collision changes the system according to

\[
\rho_S((n+1)\delta t) = \text{Tr}_A \left[ \hat{U}(\delta t) (\rho_S(n\delta t) \otimes \rho_A) \hat{U}^\dagger(\delta t) \right],
\]

where \(\rho_A\) is the state of the \(n\)-th auxiliary unit and where the unitary operator is given by

\[
\hat{U}(\delta t) = e^{-i\delta t(\hat{H}_S + \hat{H}_A + \hat{H}_{SA})}.
\]

Here and throughout, we chose units such that \(\hbar = 1\). As we will discuss in more detail in Section III, this picture allows us to neatly define and compute all the thermodynamic quantities such as heat, work, and entropy production, for arbitrary system-environment interactions. It is known that we can write down a master equation in GKSL form for the open system’s evolution [27, 29]. As such, one would naively expect that the corresponding thermodynamics would follow from the traditional formalism, see, e.g., Ref. [30, 31], whereby all of the relevant quantities can be determined from the system state. However, as we discuss in the following, such a picture is only valid when the system-environment interaction is energy-preserving (i.e., it is in the rotating wave form), which is the only type of interaction where an equilibrium steady state. However, as we discuss in the following, such a picture is only valid when the system-environment interaction is energy-preserving (i.e., it is in the rotating wave form), which is the only type of interaction where an equilibrium steady state (ESS) is achieved. Any other form of interaction gives rise to a NESS, which is maintained via steady state currents due to the energy invested in switching on and off the interaction in Eq. (1).

**A. Continuous time limit**

Let us consider the most general interaction Hamiltonian of the form \(\hat{H}_{SA} = g\hat{V}_{SA} = g \sum_{i,j} \hat{S}_i \otimes \hat{A}_j\), where \(g\) is a common rescaling constant denoting the intensity of the coupling and where \(\hat{S}_i, \hat{A}_j\) are generic system (environmental unit) operators. Note that, in general, \(\hat{V}_{SA}\) does not commute with \(\hat{H}_S\). Following [32–34], it is convenient to assume that the coupling constant is proportional to the collision time according to \(g \propto (\delta t)^{-1/2}\). We also assume that \(\hat{H}_S = J \sum_i \hat{S}_i\), where the system’s characteristic frequency, \(J\), sets the intrinsic system evolution timescale \(t_S = J^{-1}\) over which the typical coherent dynamics generated by \(\hat{H}_S\) occurs. Furthermore, without any loss of generality [5, 29], we assume that all the odd moments of the interaction Hamiltonian, \(\hat{H}_{SA}\), have zero average, i.e., \(\text{Tr}_A (\hat{H}_{SA}^{2n+1} \rho_A) = 0\). Finally, as stated above, we take \(t_S \ll \delta t\), or, equivalently, \(J \delta t \gg 1\); we are, thus, justified in neglecting the system’s evolution between subsequent collisions. However, this does not mean that the system’s free Hamiltonian is irrelevant, as it can play a crucial role during the interaction time [29].

We briefly recall, here, the derivation provided in Refs. [27, 29], where it has been shown that a closed effective master equation for the dynamics of the reduced system in the short collision time regime, \(\delta t \ll 1\), is obtainable. Moving to the interaction picture with respect to \(\hat{H}_A\), and expanding the unitary evolution operator (3) up to second order in \(\delta t\), with \(g = g_0 \delta t^{-1/2}\), leads to

\[
\hat{U}(\delta t) \simeq \mathbb{1}_{SA} - i \left( \hat{H}_S + \frac{g_0}{\sqrt{\delta t}} \hat{V}_{SA} \right) \delta t - \frac{g_0^2}{2\delta t} \hat{V}_{SA}^2 \delta t^2,
\]

Substituting Eq. (4) into Eq. (2) leads to the approximate expression for the change of the system’s state due to a single collision

\[
\frac{\delta \rho_S(n\delta t)}{\delta t} = \rho_S((n+1)\delta t) - \rho_S(n\delta t) = -i \left[ \hat{H}_S, \rho_S(n\delta t) \right] + \frac{g_0^2}{2} \text{Tr}_A \left[ \hat{V}_{SA} (\rho_S(n\delta t) \otimes \rho_A) \hat{V}_{SA}^\dagger \right] + \frac{g_0^2}{4} \text{Tr}_A \left[ \left\{ \hat{V}_{SA}^\dagger \hat{V}_{SA}, (\rho_S(n\delta t) \otimes \rho_A) \right\} \right] = \frac{g_0^2}{2} \text{Tr}_A \left[ \hat{V}_{SA}^\dagger \hat{V}_{SA}, (\rho_S(n\delta t) \otimes \rho_A) \right] - \frac{g_0^2}{2} \text{Tr}_A \left[ \hat{V}_{SA}, (\rho_S(n\delta t) \otimes \rho_A) \hat{V}_{SA}^\dagger \right] = \frac{g_0^2}{2} \text{Tr}_A \left[ \hat{V}_{SA}^\dagger \hat{V}_{SA}, (\rho_S(n\delta t) \otimes \rho_A) \right] = \sum_{jk} \gamma_{jk} \left( \hat{S}_j \rho_S(n\delta t) \hat{S}_k^\dagger - \frac{1}{2} \left\{ \hat{S}_k^\dagger \hat{S}_j, \rho_S(n\delta t) \right\} \right),
\]

where the explicit (but generic) form for \(\hat{V}_{SA}\) introduced above has been used to obtain the last line, while \(\gamma_{jk} = g_0^2 \text{Tr}_A \left[ \hat{A}_k^\dagger \hat{A}_j \right] \) is the damping rate determined by the environmental auto-correlation function [29]. Taking the continuous time limit \(\lim_{\delta t \to 0^+, n \to +\infty} \frac{\delta \rho_S(n\delta t)}{\delta t} = \frac{d\rho_S(t)}{dt}\), with \(t = n\delta t\) being finite, finally allows us to obtain the master equation

\[
\frac{d\rho_S(t)}{dt} = -i \left[ \hat{H}_S, \rho_S(t) \right] + \mathcal{L}(\rho_S(t)),
\]

where the dynamical generator is in GKSL form

\[
\mathcal{L}(\rho_S(t)) = \sum_{jk} \gamma_{jk} \left( \hat{S}_j \rho_S(t) \hat{S}_k^\dagger - \frac{1}{2} \left\{ \hat{S}_k^\dagger \hat{S}_j, \rho_S(t) \right\} \right).
\]

Note that the convenient rescaling we have chosen for the interaction \(\hat{H}_{SA} = g\hat{V}_{SA}\) with \(g \propto (\delta t)^{-1/2}\) implies that the GKSL master equation, Eq. (6), has been derived in the ultra-strong coupling regime. In other words, since it is valid for \(\delta t \to 0^+\), it requires a diverging coupling strength to ensure a meaningful contribution from the system-environment interaction. Such an approach in deriving a GKSL master equation, alongside the familiar weak coupling Born-Markov-secular approximation [5], is called singular coupling limit [6], which corresponds to the case at hand where the environmental correlation function is \(\delta\)-correlated in time.

The structure of Eq. (6) for the generator of the reduced dynamics has several important consequences. It guarantees that the dynamical map \(\rho_S(0) \mapsto \rho_S(t) = \Lambda(t, 0)[\rho_S(0)]\),
with \( \Lambda(t, 0) = e^{tL} \), is completely positive and trace preserving, thus representing a physical operation. Furthermore, it implies semigroup composition law \( \Lambda(t, s) \Lambda(s, 0) = \Lambda(t, 0) \).

This, in turn, characterizes the dynamics as Markovian, i.e. memoryless, according to all of the criteria introduced in the literature [35]. Additionally, it guarantees the existence of a unique fixed point \( \rho^* \), satisfying the condition \( \mathcal{L}(\rho^*) = 0 \). This ensures that there is a well defined steady-state for all kind of interactions. The investigation of the properties of these steady-states is the primary focus of the present work.

There are manifestly two categories of such states: equilibrium steady states (ESS) and non-equilibrium steady states (NESS). A principle difference between the two is the presence of non-zero average entropy production for NESS. This implies that these states support non-zero currents for thermodynamic quantities. When the environment, or each auxiliary unit of the stream, is considered to start in a KMS state, such as a thermal state \( \rho_A \equiv \rho_A^\beta = Z_A^{-1} e^{-\beta H_A} \) with \( Z_A = \text{Tr} \left[ e^{-\beta H_A} \right] \), then the so-called KMS condition for the decay function \( \gamma_{jk}(-\omega) = e^{-\beta \omega} \gamma_{kj}(\omega) \) is satisfied. The latter, when combined with a GKSL master equation derived under the secular approximation, which decouples the evolution of the populations from that of the coherences, leads to detailed balance. This implies that the stationary state is the thermal state \( \rho^* \equiv \rho^*_S = Z_S^{-1} e^{-\beta H_S} \). Thus, thermal equilibration with the bath is achieved, and the system reaches the ESS.

Crucially however, in our case the master equation Eq. (6) in GKSL form was obtained without performing the secular approximation, owing to the rescaling of the system-environment interaction Hamiltonian, which brought us to the singular coupling regime. Therefore, the equations of motion for the populations and the coherences are not necessarily decoupled from each other, and this means that even if the state of the environment satisfies the KMS condition, the detailed balance is not fulfilled and, therefore, the stationary state is given by some form of NESS. In the following Sections, we will characterize the types of achievable NESS, showing that we can even reach stationary states with non-zero values of coherences in the system’s energy eigenbasis. We will show that, at least for the class of collision models we considered, an ESS is reached only when the system-environment interaction is energy preserving, which is the only choice of system-environment interaction for which the aforementioned equations of motion do indeed decouple, so that one ends up with \( \rho^* = \rho^*_S \). On the other hand, all other forms of interactions lead to a NESS. As a consequence, we show below that one must carefully account for the switching on and off of the interaction term in order to accurately capture the thermodynamics of the process in these cases.

### III. THERMODYNAMICS OF OPEN QUANTUM SYSTEMS

Consider the typical setting of a system with Hamiltonian \( \hat{H}_S(t) \), interacting with an environment with Hamiltonian \( \hat{H}_E \) via a coupling term \( \hat{H}_{SE}(t) \). The time-dependence in \( \hat{H}_S(t) \) and \( \hat{H}_{SE}(t) \) is assumed to arise due to some external control protocol, and therefore acts only at the level of the system, which usually incorporates the controllable degrees of freedom. The overall dynamics is governed by the unitary operator

\[
U(t) = \frac{1}{\mathcal{T}} \exp \left[ -i \int_0^t d\tau \hat{H}_{tot}(t) \right],
\]

with \( \hat{H}_{tot}(t) = \hat{H}_S(t) + \hat{H}_E + \hat{H}_{SE}(t) \). Assume, further, that system and environment are initially uncorrelated, i.e. \( \rho_{SE}(0) = \rho_S(0) \otimes \rho_E(0) \), and, in order to meaningfully study the thermodynamic properties, that the environment is a thermal bath with a generic inverse temperature \( \beta \in [-\infty, +\infty] \).

\[
\rho_E(0) = \rho_E^\beta \equiv Z_E^{-1} e^{-\beta \hat{H}_E} \]  

where \( Z_E = \text{Tr}_E \left[ e^{-\beta \hat{H}_E} \right] \).

The work performed by the external agent responsible for the explicit time dependence of the Hamiltonian can be defined as the change in the total energy of the composite system, induced by the action of the external protocol

\[
W(t) = \text{Tr}_{SE} \left[ \hat{H}_{tot}(t) \rho_{SE}(t) - \hat{H}_{tot}(0) \rho_{SE}(0) \right] = \int_0^t d\tau \frac{d}{d\tau} \left( \text{Tr}_{SE} \left[ \hat{H}_{tot}(\tau) \rho_{SE}(\tau) \right] \right) = \int_0^t d\tau \text{Tr}_{SE} \left[ \left( \frac{d\hat{H}_{tot}(\tau)}{d\tau} + \frac{d\hat{H}_{SE}(\tau)}{d\tau} \right) \rho_{SE}(\tau) \right] \quad (9)
\]

where we have used

\[
\text{Tr}_{SE} \left[ \hat{H}_{tot}(\tau) \frac{d\rho_{SE}(\tau)}{d\tau} \right] = 0 \quad (10)
\]

since \( \frac{d\rho_{SE}(\tau)}{d\tau} = -i \left[ \hat{H}_{tot}(\tau), \rho_{SE}(\tau) \right] \) and due to the assumption that the Hamiltonian of the environment is time independent. The heat can be analogously defined as the change in the energy of the bath [36, 37],

\[
Q(t) = \text{Tr}_E \left[ \hat{H}_E(\rho_E(t) - \rho_E(0)) \right] = \int_0^t d\tau \text{Tr}_E \left[ \hat{H}_E \frac{d\rho_E(\tau)}{d\tau} \right]. \quad (11)
\]

As the overall system is considered closed, its evolution is unitary and the first law of thermodynamics is satisfied. From Eqs. (9) and (11) the change in the internal energy is

\[
\Delta E(t) = \text{Tr}_{SE} \left[ (\hat{H}_S(t) + \hat{H}_{SE}(t)) \rho_{SE}(t) \right] - \text{Tr}_{SE} \left[ (\hat{H}_S(0) + \hat{H}_{SE}(0)) \rho_{SE}(0) \right] = \int_0^t d\tau \frac{d}{d\tau} \left( \text{Tr}_{SE} \left[ (\hat{H}_S(\tau) + \hat{H}_{SE}(\tau)) \rho_{SE}(\tau) \right] \right),
\]

(12)
which is well-defined independently of the strength of the coupling between system and bath. At the level of the second law, one finds that the entropy production is given by

\[ \Sigma(t) = \beta Q(t) - \Delta S(t) = D(\rho_{SE}(t)) \| \rho_S(t) \otimes \rho_E^n \), \]

where \( \Delta S(t) = S(\rho_S(t)) - S(\rho_{SE}(t)) \) is the change in the system’s von Neumann entropy \( S(\rho) = -\text{Tr} [\rho \ln \rho] \), and where \( D(\rho||\sigma) = \text{Tr}[\rho \ln \rho] - \text{Tr}[\rho \ln \sigma] \) is a relative entropy. In Refs. [36, 37] it has been shown that the irreversible entropy production can be equivalently calculated as

\[ \Sigma(t) = I(\rho_S(t), \rho_E(t)) + D(\rho_E(t)||\rho_E^n), \]

where \( I(\rho_S(t), \rho_E(t)) \equiv S(\rho_S(t)) + S(\rho_E(t)) - S(\rho_{SE}(t)) \) is the mutual information between the system and the environment (see also Refs. [38, 39]). This expression shows that two terms contribute to the entropy production, one is correlation between \( S \) and \( E \) built up during the coupled evolution and the other is the change in the environmental state. The application of Klein’s inequality [5] immediately leads to the conclusion that the entropy production is a positive quantity. Its time derivative however, i.e. the entropy production rate, is not generally constrained to be positive. Transient non-Markovian dynamics is known to lead to negative entropy production rates [40–43] although a strict relationship between these notions is still lacking [44, 45].

A. Weak coupling limit

Taking one extreme of the singular coupling limit, i.e., the oft-considered weak coupling limit, where the interaction Hamiltonian \( \hat{H}_{SE} \) is proportional to a coupling constant that is much smaller than any energy scale of \( \hat{H}_S \) and \( \hat{H}_E \), we find that the work, Eq. (9), reduces to

\[ W(t) \simeq \int_0^t d\tau \text{Tr}_{SE} \left( \frac{d\hat{H}_S(\tau)}{d\tau} \rho_{SE}(\tau) \right) \]

\[ = \int_0^t d\tau \text{Tr}_S \left( \frac{d\hat{H}_S(\tau)}{d\tau} \rho_S(\tau) \right) \]

(15)

and the change in the internal energy is

\[ \Delta E(t) \simeq \int_0^t d\tau \frac{d}{d\tau} \left( \text{Tr}_S \left[ \hat{H}_S(\tau) \rho_S(\tau) \right] \right) \]

(16)

From the first law, it then, follows that the heat is given by

\[ Q(t) \simeq \int_0^t d\tau \text{Tr}_S \left[ \hat{H}_S(\tau) \frac{d}{d\tau} (\rho_S(\tau)) \right], \]

(17)

all of which is consistent with the standard definitions put forward in [30]. Note that the last expression could be equivalently derived from Eq. (11) by writing \( \hat{H}_E = \hat{H}_{tot} - \hat{H}_S - \hat{H}_E \), neglecting the last term due to the weak coupling approximation and using Eq. (10). This implies that, in the weak-coupling limit, all of the thermodynamic quantities can be calculated directly from the reduced system only, once the generator of the dynamics is known. Indeed, the entropy production, in this limit, can be written as \( \Sigma(t) = \int_0^t d\tau \sigma(\tau) \), with the rate \( \sigma \) given by

\[ \sigma(t) = \frac{d}{dt} (\Delta S(t) - \beta Q(t)) \]

\[ = -\text{Tr}_S \left[ \frac{d}{dt} \rho_S(t) \left( \ln \rho_S(t) + \beta \hat{H}_S \right) \right]. \]

(18)

Using the thermal state of \( S, \rho_S^\text{th} \), we could have finally rewritten the above expression as

\[ \sigma(t) = \frac{d}{dt} D(\rho_S(t)||\rho_S^\text{th}). \]

(19)

When \( \rho_S^\text{th} \) is the stationary state of the dynamics, i.e. \( \frac{d\rho_S^\text{th}}{dt} = 0 \), which occurs when the Born-Markov and secular approximations are assumed to be valid, in addition to the weak-coupling limit, leading to a master equation in GKSL form, then Spohn’s inequality [31] guarantees that \( \sigma(t) \geq 0 \) \( \forall t \).

We stress that Eqs. (15), (16), (17) and (19) are valid only in the weak coupling regime. As we will establish, despite the dynamics being described by a master equation with the same general form, these expression cannot be applied verbatim to describe the thermodynamics of collision models considered in this work.

B. Thermodynamics of collisional models

Returning to the collision models described by Eq. (2), we remark that, while we do not consider any explicit time dependence in the system’s Hamiltonian, the full system-environment interaction is in fact time dependent by virtue of Eq. (1). We will find that this is the sole source of work that maintains generic NESS. We assume all environmental units to be initially prepared in the Gibbs thermal state \( \rho_A^\text{th} \). Evaluating Eq. (9) over a single collision, then, gives us an expression for the energetic cost which can be written in terms of the work required to switch on and off the interaction Hamiltonian

\[ W(\delta t) = \text{Tr}_{SA} \left[ (\hat{U}^\dagger(\delta t) \hat{H}_{SA} \hat{U}(\delta t) - \hat{H}_{SA}) \rho_S(0) \otimes \rho_A^\text{th} \right] \]

(20)

This term can only vanish when the interaction commutes with the free Hamiltonian, which occurs only for the energy-preserving case typically considered in the literature [24]. Analogously, the heat dissipated into an environmental unit during a single collision is

\[ Q(\delta t) = \text{Tr}_{SA} \left[ (\hat{U}^\dagger(\delta t) \hat{H}_A \hat{U}(\delta t) - \hat{H}_A) \rho_S(0) \otimes \rho_A^\text{th} \right]. \]

(21)

The change in the internal energy after each collision as well as the entropy production follow immediately, where in particular \( \Delta \Sigma(\delta t) = \Delta S(\delta t) - \beta Q(\delta t) \), with \( \Delta S(\delta t) \equiv S(\rho_S(\delta t)) - S(\rho_S(0)) \). Notice that we have made use of the fact that for the memoryless collision model with fixed \( \delta t \) these quantities do not depend on the specific collision, \( n \).
It is interesting and instructive to consider how Eqs. (20) and (21) change in the continuous time limit $n \to \infty$ and $\delta t \to 0^+$ such that $t \equiv n \delta t$ is finite, which corresponds to the other extreme of the singular coupling limit, the ultra-strong coupling limit, where the evolution of the reduced system is also governed by a master equation in GKSL form, Eq. (5). In this limit, Eqs. (20) and (21) can be simplified by using Eq. (4), leading to $W(t) = \int_0^t d\tau \dot{W}(\tau)$ and $Q(t) = \int_0^t d\tau \dot{Q}(\tau)$ with

\[
\dot{W}(t) \equiv \lim_{\delta t \to 0^+} \frac{W(\delta t)}{\delta t} = \text{Tr}_{SA} \left[ \left( \hat{H}_{SA} (\hat{H}_S + \hat{H}_A) \right) \hat{H}_{SA} - \frac{1}{2} \left\{ \hat{H}_{SA}^2, (\hat{H}_S + \hat{H}_A) \right\} \right] \rho_S(t) \otimes \rho_A^b ,
\]

\[
\dot{Q}(t) \equiv \lim_{\delta t \to 0^+} \frac{Q(\delta t)}{\delta t} = \text{Tr}_{SA} \left[ \left( \hat{H}_{SA} \hat{H}_A \hat{H}_{SA} - \frac{1}{2} \left\{ \hat{H}_{SA}^2, \hat{H}_A \right\} \right) \rho_S(t) \otimes \rho_A^b \right] .
\]

Finally, when the system has reached the steady-state the changes in both the internal energy $\Delta U(t)$ and the entropy $\Delta S(t)$ will vanish, while work and heat will become equal and opposite. In the cases where the interaction is energy preserving, the steady-state $\rho^*$ will be the thermal state $\rho_S^\beta$, and, consequently, both heat and work will vanish, too. This is the only situation where thermal equilibrium is reached. For any other interaction Hamiltonian that does not preserve the bare energy $\hat{H}_S + \hat{H}_A$, a NESS is attained, which supports finite heat and work currents. Once integrated, these quantities provide an elegant example of the so-called housekeeping heat and work [46-48], which are necessary to maintain the steady-state out of equilibrium. These quantities, if calculated over an infinite time interval, diverge linearly as a result of the fact that the currents become constants in the steady-state. In the following, we will elucidate these results for paradigmatic interactions.

IV. EXEMPLARY CASE STUDY: QUBIT COLLISION MODEL

We will consider the system and all auxiliary units to be two-level quantum systems, with their respective free Hamiltonians given by $\hat{H}_{SA}(t) = \omega(t) A^\dagger A + \sum_i \hat{\sigma}_i$, where $\{ \hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z \}$ are the usual Pauli matrices. We chose the generic two-body interaction

\[
\hat{H}_{SA} = \sum_{lm} J_{lm} \hat{\sigma}_l \otimes \hat{\sigma}_m .
\]

As our focus is on steady state properties, which are independent of the choice of the initial system state, without any loss of generality, in what follows, we will assume an arbitrarily chosen $\rho_S(0)$. While quantitative differences occur transiently, the qualitative behavior exhibited holds for any other suitable choice of initial state. The environmental qubits are prepared in the Gibbs state $\rho_A(0) = \rho_A^b$ with

\[
\rho_A^b = \begin{pmatrix} \frac{1}{2} \left[ 1 - \tanh \left( \frac{\beta \omega_A}{2} \right) \right] & 0 \\ 0 & \frac{1}{2} \left[ 1 + \tanh \left( \frac{\beta \omega_A}{2} \right) \right] \end{pmatrix},
\]

and $\rho_{SE}(0) = \rho_S(0) \otimes \rho_A^b$. In the following numerical results, the continuous time limit is achieved by taking the collision time $\delta t \sim 5 \times 10^{-2} \omega_S$ and $n = 5000$, such that $t = n \delta t = 250 \omega_S$. This guarantees that we are well within the steady-state regime dictated by the master equation.

A. Diagonal steady states in the energy eigenbasis

Let us start by considering the diagonal interaction case, i.e.

\[
\hat{H}_{SA} = J_x \hat{\sigma}_x \otimes \hat{\sigma}_x + J_y \hat{\sigma}_y \otimes \hat{\sigma}_y ,
\]

where the term $\propto \hat{\sigma}_z \otimes \hat{\sigma}_z$ has been neglected as it essentially amounts to a simple phase factor. When $J_x = J_y$, and the system and auxiliary qubits are resonant, i.e. $\omega_S = \omega_A$, the interaction is energy preserving, and, therefore, we have vanishing heat and work currents at the steady-state

\[
\dot{W}(t) = \dot{Q}(t) = 0 .
\]

The resulting stationary state is the equilibrium Gibbs distribution at the same inverse temperature $\beta$ of the environment, meaning that we achieved an ESS. This is the only interaction for which Eqs. (15), (16), (17) and (19) accurately capture the thermodynamics of the process and constitute the type of interaction typically considered in the literature [12, 13, 15, 18, 19, 22, 24].

For any other setting governed by Eq. (26) the system will reach a NESS, $\rho^*$, which is diagonal in the energy eigenbasis. As our system is a qubit, it is possible to express the steady-state as a Gibbs state at an effective inverse temperature $\beta_{\text{eff}}$ such that

\[
\rho^* = \rho_S^b(\beta_{\text{eff}}) = \frac{e^{-\beta_{\text{eff}} \hat{H}_S}}{\text{Tr}_S [e^{-\beta_{\text{eff}} \hat{H}_S}]}.
\]

In particular, for a balanced but off-resonance scenario, i.e. $J_x = J_y$ but $\omega_S \neq \omega_A$, $\beta_{\text{eff}}$ can be found simply through the relation $\beta_{\text{eff}} \omega_S = \beta \omega_A$. Therefore, this situation essentially amounts to a re-normalization of the effective temperature.

A more interesting situation occurs when both system and environmental units are resonant and $J_x \neq J_y$. In this case,
the effective temperature has a more involved dependence as a function of the ratio $J_y/J_x$. In Fig. 1(a) the various curves correspond to different bath temperatures, with the gradient from lighter-blue to darker-red corresponding to increasing temperature. For $J_y/J_x = 0$ the steady state has an infinite effective temperature, $\beta_{\text{eff}} = 0$, meaning that the stationary state $\rho^*$ is the maximally mixed state. For $J_y/J_x < 1$, $\beta_{\text{eff}}$ increases with the ratio of the coupling strengths $J_y/J_x$, eventually reaching thermal equilibrium only when $J_y/J_x = 1$. Further increasing the ratio, $J_y/J_x > 1$, the steady-state temperature increases, and it asymptotically approaches zero as $J_y/J_x \to \infty$. Notice that $|\beta_{\text{eff}}| < 1$ for all the possible values of coupling strengths $J_y/J_x$. This indicates that the system is always driven to a higher effective temperature than the bath. We also see that cold environments maintain NESS that are further away from equilibrium, relative to the bath temperature. Interestingly, when $J_y$ and $J_x$ have different signs, i.e. $J_y/J_x < 0$, the system settles to a NESS with inverted populations, indicated by a negative $\beta_{\text{eff}}$. This behavior is present for all initial environment temperatures and, importantly, does not require the auxiliary qubits to be inverted, it is solely controlled by $\hat{H}_{SE}$. The crucial difference between these NESS and those that attain a positive temperature is that the former are active states [49]. Therefore, work can be extracted from them via unitary cyclic processes [50–53].

Turning our attention to the thermodynamic quantities, through Eqs. (20) and (21), we show the work, heat, and entropy production in Fig. 1 as insets of their respective currents, as a function of time $t = n\Delta t$, for different choices of $J_y/J_x$ and for resonant system and environment $\omega_S = \omega_A$. When the system-environment interaction preserves the total energy, i.e. $J_y = J_x$ (solid curves), the energetic cost of switching the interaction on and off vanishes as evidenced in Fig. 1(b), where both the work and its current remain zero throughout. During the transient, panel (c) shows that a finite amount of heat enters the system, thermalizing it to the environment temperature, and, therefore, bringing the system to the ESS. The entropy production behaves consistently with these findings, and, crucially, we observe that both heat and entropy currents vanish in the steady-state regime, as the system has reached the ESS. This is consistent with the fact that, in this case, system and environment return to a fully factorized state [54].

Shifting our focus to the unbalanced interactions, we find the underlying mechanisms supporting the NESS. From Fig. 1, it is clear that for such interactions the steady-state heat, work and entropy production have constant, non-zero currents. Therefore, all of these quantities keep changing linearly with time. The currents that remain in the steady-state are clear examples of housekeeping heat and work that keep the system out of the equilibrium [46–48]. Since the system-environment interaction does not preserve the total energy, it is the work associated to switching the interaction on and off between consecutive collisions that is the source for supporting the NESS. We find that higher effective temperatures for the system imply larger heat, work and entropy currents, with the maximum occurring for $J_y/J_x = 0$ (dot-dashed). Thus, the magnitude of housekeeping currents increases when the system is kept further out of equilibrium with respect to the bath.

### B. Coherent non-equilibrium steady states

Finally, we examine the possibility to generate steady-states with coherence in the energy eigenbasis. Our interest is twofold: first, the interaction of a quantum system with its environment generally results in the loss of its quantum properties; therefore introducing a way of achieving coherence in an open system setting is interesting in its own right. Second, from the thermodynamic point of view, similarly to the NESS at a negative temperature discussed previously, steady-states with coherence are also non-passive and, therefore, work can be extracted from them [55].

Owing to the generality of the system-environment interaction in the derivation of our master equation we find that generating steady-state coherence (SSC) is possible for interaction Hamiltonians of the form

$$\hat{H}_{SA} = J_z \hat{\sigma}_z \otimes \hat{\sigma}_x + J_y \hat{\sigma}_z \otimes \hat{\sigma}_y.$$  \hfill (29)
Notice that this Hamiltonian belongs to the class of interactions put forward in Ref. [56], as it consists of both a parallel term with respect to $\hat{H}_S$, $\hat{\sigma}_z \otimes \hat{\sigma}_y$, and a perpendicular one, $\hat{\sigma}_x \otimes \hat{\sigma}_x$. In order to quantify the amount of coherences, we will employ the $l_1$ norm of coherence $C = \sum_{l \neq m} |\rho_{lm}|$, first introduced in [57], which can be shown to satisfy all the properties to be considered as a valid coherence measure [58].

Fig. 2(a) shows its dependence on $\alpha = \arctan(J_{yz}/J_x)$, for different environment temperatures. When either of the two couplings goes to zero, the SSC vanish, cf. Fig. 2(a). Furthermore, in agreement with the results obtained in [56, 59], the maximum amount of SSC is obtained when $\alpha = \pi/4$ and for zero temperature environments. The amount of SSC monotonically decreases with increasing bath temperature.

Turning to Fig. 2(b)-(d), we see that, regardless of the value of $\alpha$, we always achieve a NESS with non-zero and opposite heat and work currents, with the asymptotic values of these currents being independent of $\alpha$. In particular, we see that these currents are not affected by switching on the SSC generating term $\propto \hat{\sigma}_x \otimes \hat{\sigma}_y$, which only induces oscillations in the transient, and, therefore, we can conclude that the steady-state thermodynamics is entirely dictated by the perpendicular term entering Eq. (29). While the steady-state currents are the same in all of the considered cases, the integrated quantities can have different values, entirely due to their transient behavior, which explicitly depends on the choice of the initial state of the system, and where the coherence can play a crucial role [39]. Therefore, if one wishes to minimize, for example, the irreversible entropy production throughout the dynamics, it is necessary to perform an optimization procedure at the initial state preparation level.

V. CONCLUSIONS

We have examined the thermodynamics of memoryless quantum collision models through a master equation description derived in the singular coupling limit, which allows our results to hold in the ultra-strong coupling regime and is valid for any system-environment interaction. By carefully examining the associated energy exchanges at play, we showed that, despite the dynamics being fully described by a master equation in GKSL form, the corresponding thermodynamics cannot be described by properties of the system alone, in contrast to the weak-coupling limit. The root of this discrepancy lies in the fact that the secular approximation is not taken and, as such, the equations of motion for populations and coherences do not decouple, with the notable exception of energy-preserving interactions, which is the only instance where the system reaches thermal equilibrium with the bath.

We have demonstrated our results for an all-qubit version of our collision model, explicitly showing that both equilibrium and non-equilibrium steady-states (NESS) are admitted by the dynamics. We have shown the rich variety of NESS that emerge, broadly falling into two distinct categories: those that are diagonal in the energy eigenbasis and those that exhibit steady-state coherences (SSC). Among the NESS achievable, those with negative effective temperatures and those with SSC particularly stand out. The former implies that it is possible to achieve a population inversion, while the latter is one of the few examples of coherence generation through an interaction with an environment. For those states exhibiting SSC, we have further established that the coherence generating part of the interaction does not contribute to the steady-state thermodynamics. These states are examples of non-passive states, and, therefore, one can extract a non-zero amount of work from them. We established that all NESS are supported by non-zero work, heat, and entropy currents. These quantities account for the cost of maintaining steady states out-of-equilibrium with the environment, and, therefore, provide an elegant demonstration of the housekeeping work and/or heat. Our work therefore contributes to the ongoing effort to understand the thermodynamics of strongly coupled quantum systems, see e.g. [60, 61].

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