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Open Quantum Evolution from Thermodynamic Collision Models

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Abstract

The framework of open quantum systems (**OQS**) is used to describe the dynamics of a quantum system interacting with its environment. In a realistic scenario, systems inevitably couple to their environment, and furthermore, given minimal knowledge of the environment, it is reasonable to assume that the system equilibrates with its environment at some time. In a thermodynamic setting, such equilibration processes are referred to as *thermalization* and can be observed ubiquitously in our everyday lives.

One key application of open quantum systems is to describe the open system dynamics with a quantum master equation (**ME**). All physically meaningful MEs take the form famously espoused by Gorini-Kossakowski-Sudarshan-Lindblad (**GKSL**) [1, 2] and Franke [3], which implies a particular structure for the possible dynamics, stemming from natural assumptions such as Markovianity. When the interaction between system and environment is energy conserving, additional restrictions apply to the GKSL equation [4], which allow one to derive properties about the system directly from the quantum master equation.

In this thesis, we take a different approach and model the open quantum system dynamics in a Markovian collision model (**CM**) based on consecutive interactions between the system and its thermal environment. We chose this approach since, a priori, it is not clear that invoking such thermodynamic assumptions on the GKSL equation leads to the same description as when these assumptions are already weaved in the construction process of a master equation. This approach provides a microscopic mechanism for the open system evolution according to thermodynamic assumptions, ensuring that the interactions follow strict energy conservation (**SEC**). Afterwards, we take the continuous-time limit to find a quantum master equation of GKSL form.

The resulting master equation shows the same structure as the one found in Ref. [4], despite different approaches. This enables us to study the similarities, such as the satisfaction of a detailed balance (**DB**) condition of the kinetic coefficients.

Additionally, the collision model approach allows computing properties, such as decay rates, in terms of relevant Hamiltonians, which offers additional insight on how thermodynamic processes can be tuned. We find that from a given detailed balance compliant master equation one can always construct at least one Hamiltonian describing the system-environment interaction that also fulfils strict energy conservation. This result allows us to study the underlying relation between detailed balance and strict energy conservation.

Kurzfassung

Das physikalische Rahmenwerk der offenen Quantensysteme (**OQS**) wird verwendet, um die Dynamik eines Quantensystems zu beschreiben, das mit seiner Umgebung interagiert. In einem realistischen Szenario koppeln Systeme unvermeidlich an ihre Umgebung. Zudem ist es bei minimalen Kenntnissen über die Umgebung vernünftig anzunehmen, dass sich das System nach einiger Zeit mit seiner Umgebung im Gleichgewicht befindet. In einem thermodynamischen Kontext werden solche Gleichgewichtsprozesse als *Thermalisierung* bezeichnet und können in unserem Alltag allgegenwärtig beobachtet werden.

Eine zentrale Anwendung der OQS besteht darin, die Systemdynamik eines offenen Systems mit einer Quantenmastergleichung (**ME**) zu beschreiben. Alle physikalisch sinnvollen ME nehmen die berühmte Form der Gorini-Kossakowski-Sudarshan-Lindblad (**GKSL**)-Gleichung an, wie sie von [1, 2] und Franke [3] formuliert wurde. Diese Struktur ergibt sich aus physikalische motivierten Annahmen wie der Markovianität. Wenn die Wechselwirkung zwischen System und Umgebung energieerhaltend ist, gelten zusätzliche Einschränkungen für die GKSL-Gleichung [4], die es ermöglichen, Eigenschaften des Systems direkt aus der ME abzuleiten.

In dieser Arbeit verfolgen wir einen Ansatz in dem wir die Dynamik offener Quantensysteme in einem Markovschen Kollisionsmodell (**CM**), die auf aufeinanderfolgenden Interaktionen zwischen dem System und seiner thermischen Umgebung basiert, modellieren. Wir haben diesen Ansatz gewählt, da es a priori nicht klar ist, ob thermodynamische Annahmen direkt auf die GKSL-Gleichung angewendet zur gleichen Beschreibung führen wie, wenn diese Annahmen bereits in der Herleitung einer Mastergleichung eingebettet sind. Dieser Ansatz liefert einen mikroskopischen Mechanismus für die zeitliche Veränderung des offenen Systems unter thermodynamischen Annahmen und stellt sicher, dass die Wechselwirkungen der strikten Energieerhaltung (**SEC**) folgen. Anschließend betrachten wir den Grenzwert infinitessimaler Zeitschrittlänge, um eine ME in der Form der GKSL-Gleichung zu erhalten.

Die Mastergleichung zeigt trotz unterschiedlicher Herangehensweisen die gleiche Struktur wie die in Ref. [4]. Dies ermöglicht es uns, Gemeinsamkeiten zu untersuchen, wie beispielsweise die Erfüllung einer detailierten Gleichgewichtsbedingung (**DB**) für die kinetischen Koeffizienten.

Darüber hinaus ermöglicht der CM-Ansatz die Berechnung von Eigenschaften wie Zerfallsraten in Bezug auf relevante Hamiltonoperatoren. Dies bietet zusätzliche Einblicke, wie thermodynamische Prozesse gezielt beeinflusst werden können. Wir zeigen, dass aus einer gegebenen DB-konformen Mastergleichung immer mindestens ein Hamiltonoperator konstruiert werden kann, der die System-Umgebung-Interaktion beschreibt und zugleich die strikte Energieerhaltung erfüllt. Dieses Ergebnis erlaubt es uns, die Beziehung zwischen DB und SEC zu untersuchen.

Acronyms

CM collision model

CPTP completely positive trace preserving

DB detailed balance

DOF degrees of freedom

GKSL Gorini-Kossakowski-Sudarshan-Lindblad

ME quantum master equation

NB Notebook

SEC strict energy conservation

OQS open quantum systems

Contents

1 Introduction

Out of the few assumptions we make in this thesis, energy conservation can be seen as the most fundamental one. This basic law of nature is one of the pillars of classical thermodynamics, a theory that describes time-independent equilibrium states based only on a few parameters, like temperature, volume and pressure. Thermodynamic systems are usually comprised of a large number of particles, which makes a description of the system on a microscopic basis virtually impossible. However, it is possible to describe these systems as an *ensemble*. The description based on only a few parameters is possible, not despite the huge size of the system, but because of it. Fluctuations of individual particles in large systems average out and microscopic effects that can be described with the theory of quantum mechanics become negligible for the overall behaviour of the ensemble.

Although quantum systems are small, some quantum effects (e.g. superconductivity and superfluidity) can also be observed in our macroscopic world. Understanding how such quantum effects manifest at a large scale is one of the goals of quantum thermodynamics, i.e. to precisely understand which quantum effects can be utilised or exploited with minimal knowledge or control of the system.

Several approaches have been taken to translate the thermodynamic laws to the quantum regime [5]. In this work, we account for the thermodynamic laws by modelling the interaction between a quantum system and its environment to be energy-conserving and the surrounding environment to be in a thermal equilibrium state.

To describe the nature of the interaction between a quantum system and its environment we employ the framework of open quantum systems (**OQS**). A physical system never exists in isolation and in this sense it always couples to its environment. This results in effects we refer to as dissipation, an energy exchange between system and environment. An infamous example of a dissipation process is well known to all of us and experienced virtually every day. A cup of hot coffee that is left on the table for too long will cool down and due to the dissipation of heat to its environment, it will reach room temperature at some point and is said to have thermalized with its environment. This ubiquitous process is inevitable and hints that dissipative systems show a tendency towards equilibrium with their environment.

One way to describe the path towards equilibrium of open quantum systems is through a quantum master equation (**ME**). This differential equation is used to describe how the system evolves in time due to the interaction with its

environment, which is assumed inaccessible. Therefore, no explicit reference to the environment is required in a ME. These equations were first formulated phenomenologically to describe processes like decay rates in the form of a balance equation [6]. This probabilistic description was then further developed to be applied to density matrices and these equations are therefore suitable to describe the dynamics of quantum states [7]. However, contrary to closed quantum systems, where the time evolution is governed in a unified way by the Schrödinger equation, there is no truly general quantum master equation to describe all open system dynamics.

It is a natural assumption, that all physically meaningful quantum master equations are Markovian and take the form famously espoused by Gorini, Kossakowski, Surdashan [1], Lindblad [2] and Franke [3], which is commonly referred to as GKSL equation. It can be derived by applying the Born-Markov assumptions, which imply that the environment is memoryless in a way that the effects of the interaction between system and environment decay very fast in the environment [7, 8]. These open quantum systems are referred to as Markovian.

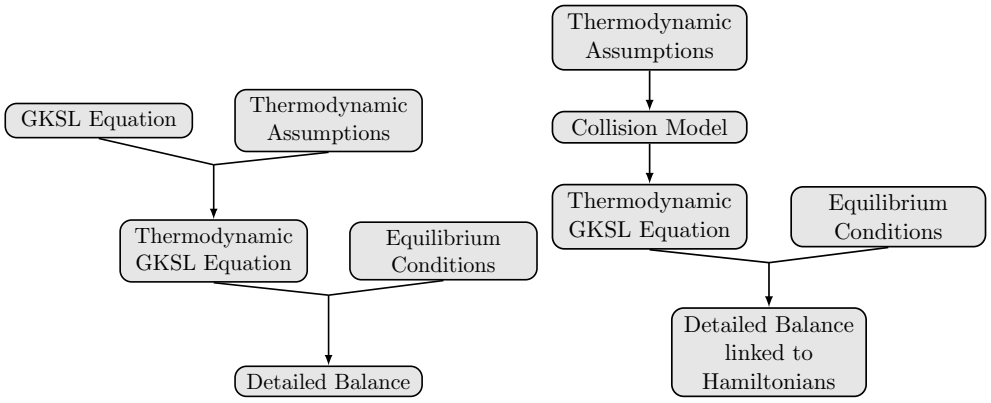
The general formulation of a GKSL equation allows for a direct study of the system properties when thermodynamic assumptions are imposed [4]. Incorporating these assumptions directly leads to a formulation of the GKSL equation that only contains thermodynamically essential terms, which allows for describing equilibration effects by a study of the ME's coefficients.

There are various non-equivalent ways to incorporate thermodynamic assumptions into open system dynamics. In this thesis, we employ a Markovian collision model, which we compare to the approach taken in Ref. [4] in Figure 1.1. The open system dynamics are modelled through consecutive collisions between system and environment, where Markovianity is implied by assuming that there are no collisions between the environment ancillas and that each environment ancilla interacts with the system only once. This inherently discrete dynamic description yields a master equation of GKSL form under taking the continuous-time limit. Additionally, the resulting equation allows for a clear connection of its coefficients and the total Hamiltonian of the open quantum system.

Originally, collision models were used to model collisions of physical particles in microwave spectroscopy [9] and in a quantum gas [10]. These models later also proved helpful in the theoretical description of a micromaser [11–13], where CMs offer a physically intuitive description of the environment composed of atoms interacting with a lossy cavity mode acting as an open system. This theoretical description then also leads to an experimental re-

alisation [14]. However, CMs are not always applied to problems linked to specific physical phenomena, sometimes they are also used as toy models in a more abstract sense. In Ref. [15] a collision model was used to find a continuous time description of a quantum system reaching its thermal equilibrium with its environment in the infinite time limit. Recently, a collision model was used to derive a quantum optics master equation [16].

In a basic Markovian collision model the interaction is modelled by consecutive collisions between system and environment particles, while the environment itself shows no internal collisions. In the approach taken in this work each of these individual collisions is based on a thermodynamic dynamical map that has the concept of strict energy conservation (**SEC**) weaved in right in its setup. At first, these consecutive interactions lead to dynamics described in discrete time steps. However, in the continuous-time limit, a ME describing the continuous system dynamics can be found. Since we implemented thermodynamic assumptions to the setup of our collision model, the found master equation then shows thermodynamic properties in that it shows the same structure as in Ref. [4], even though they implied thermodynamic assumptions to a GKSL equation instead of considering them in the derivation of the equation. We find these two approaches to be fundamentally different and point out the similarities and differences in a discussion in Section 4.1.1.



(a) Approach of Ref. [4] **(b)** Collision model approach

Figure 1.1: In the approach of Ref. [4] (a) the thermodynamic assumptions are applied to a GKSL equation, while in the collision model approach (b), we applied the thermodynamic assumptions directly into the collision model to get a thermodynamic GKSL equation.

Additionally, through the approach via the CM, we gained insight into the structure of the master equation due to the clear connection between its coefficients and the total Hamiltonian. By applying the found formalism to

equilibrium conditions we were able to set these kinetic coefficients into a ratio to result in a detailed balance (**DB**) condition.
Since we are also able to link the coefficients in the DB condition to the total Hamiltonian of system and environment we can study the relationship between detailed balance and strict energy conservation in more detail. This study leads to the result that it is always possible to construct at least one total Hamiltonian that follows from a given detailed balance-compliant quantum master equation that then also fulfils strict energy conservation. While our approach always leads to detailed balance, when assuming that strict energy conservation holds, this result shows that the opposite direction is also true under a certain construction.
However, this one construction method is not the only one that allows for this underlying connection between detailed balance and strict energy conservation, which allows for further investigations. In the outlook of this work, we highlighted some paths that could lead to a deeper understanding of how these two concepts are linked to each other.
In this work we focused on Markovian systems that are characterised by a memoryless environment, which means that the environment is barely affected by the interactions it already had with the system. Therefore, the environment forgets about these interactions very quickly, which motivates referring to these setups as memoryless. However, the effect the interaction with the system has on the environment cannot always be neglected. The CM approach allows for implementing memory in the environment to the setup. This extends the model to Non-Markovian collision models, which are well tailored for introducing memory effects, while traditional construction methods of quantum master equations only offer tedious ways of implementing memory. We end this thesis by showcasing how our Markovian collision model can be extended to take account of these memory effects and what the next steps towards a non-Markovian thermodynamic quantum master equation look like.

2 Framework

In this section, we will introduce the key concepts to describe the time evolution of open quantum systems (**OQS**) interacting with their environment. After introducing the basic formalism of quantum mechanics, we will present the fundamentals of OQS, and quantum master equation (**ME**)s, which govern the time evolution of open systems. Next, we set up a basic collision model (**CM**), leading to a dynamic description based on a ME. In the final part of this Section, we will equip this CM with thermodynamic assumptions. Followed by Section 3 where we further investigate the effects these assumptions have on the structure of the ME.

2.1 Open Quantum Systems

Before we get started with describing open system dynamics we introduce the basics of quantum mechanics in closed systems in a finite Hilbert space of dimension d.

2.1.1 Closed Quantum Systems

Quantum States

The state of a system in quantum mechanics is described by a vector ψ in a Hilbert space $\mathbb{H}$. We consider finite-dimensional Hilbert spaces, e.g $\mathbb{H} = \mathbb{C}^d$, where d is the dimension of the complex vector space.

The bra-ket formalism (or Dirac notation) is typically used in quantum mechanics to describe these states. In this formulation, a pure quantum state is represented by a ket $|\psi_i\rangle \in \mathbb{H}$ and its dual by a bra $\langle\psi_i| \equiv |\psi_i\rangle^\dagger$, which is the conjugate transpose of the ket.

A Hilbert space $\mathbb{H}$ is equipped with a scalar product that is used to normalize the quantum state vector $|\psi_i\rangle$. The normalization condition can be expressed in terms of the inner product

$$||\psi_i|| = \langle\psi_i|\psi_i\rangle^{1/2} = 1. \tag{2.1}$$

The inner product is also used to define the orthogonality of quantum states, by

$$\langle\psi_i|\psi_j\rangle = \delta_{ij}. \tag{2.2}$$

With these definitions the Hilbert space is a finite dimensional complex vector space over $\mathbb{C}$ that is complete by definition of the norm in Eq. (2.1).

Linear Operators

Observables describe physical processes in quantum mechanics and are represented by linear operators acting on the elements of the Hilbert space $\mathbb{H}$. A linear operator $A : \mathbb{H} \to \mathbb{H}$ satisfies linearity

$$A(\alpha |\psi\rangle + \beta |\varphi\rangle) = \alpha A |\psi\rangle + \beta A |\varphi\rangle \;\; \forall |\psi\rangle, |\varphi\rangle \in \mathbb{H}, \;\; \alpha, \beta \in \mathbb{C}. \tag{2.3}$$

Basis Elements

A basis is an essential framework to deal with quantum states in a mathematical sense. It is composed of basis elements, that are fundamental for representing quantum states and operators in a systematic way.

A state vector $|\psi\rangle \in \mathbb{H}$ can be expressed in a complete set of basis elements $\{|i\rangle\}_{i=0}^{d-1}$ as

$$|\psi\rangle = \sum_i c_i |i\rangle . \tag{2.4}$$

Here c_i are complex coefficients depending on the chosen set of basis elements $|i\rangle$.

In this work, we restrict ourselves to bounded operators and finite-dimensional Hilbert spaces. Therefore, linear operators A can be expressed in terms of these basis elements by

$$A |j\rangle = \sum_i a_{ij} |i\rangle \;\; \text{where } a_{ij} = \langle i|A|j\rangle . \tag{2.5}$$

Similarly, the operator can also be expressed in terms of the basis elements, such that

$$A = \sum_{i,j} a_{ij} |i\rangle \langle j| \tag{2.6}$$

This notation allows for expressing operators in terms of matrices, where each matrix element a_{ij} is assigned to the respective basis elements by the operator $|i\rangle \langle j|$. In this representation one can group the matrix elements into diagonal elements ($i = j$) and off-diagonal elements ($i \neq j$).

Commutation Relations

As opposed to scalar multiplication, which commutes, operators do not necessarily show that behaviour, which can be seen on the hand of the commutator

$$[A, B] \equiv AB - BA. \tag{2.7}$$

Operators A and B are said to commute if $[A, B] = 0$, which means that the physical observables are simultaneously diagonalizable and share a common

set of non-trivial eigenvectors.
One important feature of commuting observables is that the commutation relation also holds for analytical functions of these linear operators, i.e.

$$[A, B] = 0 \Rightarrow [f(A), g(B)] = 0 \qquad \forall f, g \text{ analytical.} \tag{2.8}$$

Similarly, we define the anti-commutator as

$$\{A, B\} \equiv AB + BA. \tag{2.9}$$

Eigenvectors and Eigenvalues
Any non-zero vector $|a\rangle$ that fulfils

$$A\,|a\rangle = \alpha\,|a\rangle\,, \tag{2.10}$$

is called an eigenvector of A with corresponding eigenvalue $\alpha \in \mathbb{C}$.

Hermitian Operators
A linear operator A is called Hermitian if it equals its adjoint

$$A = A^\dagger. \tag{2.11}$$

The adjoint or equivalently conjugate transpose operator $A^\dagger$ to A can be defined by the inner product

$$\langle A\psi|\phi\rangle = \left\langle \psi|A^\dagger\phi \right\rangle \text{ where } A^\dagger := (A^*)^T \tag{2.12}$$

Each physical observable in quantum mechanics is described by a Hermitian operator. These observables have the property that they have real-valued measurement outcomes. These outcomes correspond to the eigenvalues of the Hermitian operator associated with this observable and can be found through the eigenvalue equation (2.10) by

$$A\,|\psi\rangle = a\,|\psi\rangle \text{ where } a \in \mathbb{R}\ \forall A = A^\dagger \tag{2.13}$$

Hamiltonians
The Hamiltonian H is a Hermitian operator. H is representative of the total energy of a quantum system and therefore also determines its dynamic evolution. This Hermitian operator's real eigenvalues ε_i correspond to the energy levels of the quantum system according to the corresponding eigenvalue

equation

$$H\left|\psi_i\right\rangle = \varepsilon_i \left|\psi_i\right\rangle \tag{2.14}$$

Therefore, the energy of the system in a given state $|\psi_i\rangle$ is represented by the expectation value of H. By multiplying $\langle\psi_i|$ from the left to Eq. (2.14) one can find the eigenenergy of H associated to the eigenstate ψ_i

$$\langle H\rangle_{\psi_i} = \langle\psi_i|H|\psi_i\rangle = \varepsilon_i \langle\psi_i|\psi_i\rangle = \varepsilon_i. \tag{2.15}$$

The difference between the energy levels ε_i are called *energy gaps* or *Bohr frequencies*

$$\omega_{ij} \equiv \varepsilon_j - \varepsilon_i. \tag{2.16}$$

Unitary Operators

Unitary operators are of fundamental importance for describing the time evolution of closed quantum systems. A unitary operator U acting on an element of a finite-dimensional Hilbert space $\mathbb{H}$ is defined by demanding that

$$UU^\dagger = U^\dagger U = \mathbb{1} \tag{2.17}$$

holds. By that property unitary transformations also preserve the inner product, such that

$$\langle U\psi|U\phi\rangle = \langle\psi|\phi\rangle \qquad \forall\left|\psi\right\rangle, \left|\phi\right\rangle \in \mathbb{H} \tag{2.18}$$

Applying Eq. (2.18) to the orthogonality condition, defined in Eq. (2.2), shows that U is orthogonality preserving and applying it to states $|\phi\rangle = |\psi\rangle$ as in Eq. (2.1) shows that it preserves the norm. These properties guarantee that unitary transformations preserve the inner product structure of the Hilbert space $\mathbb{H}$ and therefore also the properties of a quantum state.

Time Evolution in Quantum Mechanics

In quantum mechanics, time dependence can be introduced on either states $|\psi\rangle$, observables A or both. Each choice is described by the so-called dynamical pictures of quantum mechanics:

- *Schrödinger Picture*
  In the Schrödinger picture, observables A remain fixed while quantum states $|\psi(t)\rangle$ evolve in time. Any observable A is therefore represented as time-independent.

- *Heisenberg Picture*
  In the Heisenberg picture, quantum states $|\psi\rangle$ are fixed, and the time evolution is represented by observables $A(t)$ that evolve according to the

unitary evolution

$$A(t) = U(t,0)AU(t,0)^\dagger.$$

- *Interaction Picture*
  In the interaction picture (or Dirac picture), the aspects of both the Schrödinger and Heisenberg pictures are combined. The state vectors $|\psi(t)\rangle$ and observables $A(t)$ both evolve in time.

Throughout this thesis, we remain in the Schrödinger picture with time-independent Hamiltonians H. The quantum states $|\psi(t)\rangle$ dynamical evolution is then governed by its Hamiltonian H according to the Schrödinger equation

$$i\hbar\frac{\mathrm{d}}{\mathrm{d}t}|\psi(t)\rangle = H|\psi(t)\rangle\,, \tag{2.19}$$

where $\hbar$ is the reduced Planck constant and is set equal to 1 from now on and will therefore be omitted in all following equations. The unitary operator $U(0,t)$ is the formal solution to the Schrödinger equation, such that

$$|\psi(t)\rangle = U(t,0)\,|\psi(0)\rangle\,. \tag{2.20}$$

For time-independent Hamiltonians H the unitary time evolution operator $U(t,0)$ in Eq. (2.20) is given by

$$U(t,0) = e^{-iHt} \equiv U. \tag{2.21}$$

It is then easy to verify that U as defined in Eq. (2.21) is indeed unitary by multiplying it with its adjoint, since $H = H^\dagger$.

Mixed Quantum States - Density Matrices

A pure state $|\psi\rangle$ is not the only way states can be described in quantum mechanics, some states need to be considered as mixed. This representation is used for describing a probabilistic mixture of pure quantum states, also known as *superposition*. A density matrix ρ is a suitable representation of pure as well as mixed quantum states.

A quantum state in density matrix form is defined in terms of a convex combination of pure state projectors $|\psi_i\rangle\langle\psi_i|$ such that

$$\rho = \sum_{i=0}^{d-1} p_i\,|\psi_i\rangle\langle\psi_i|\,. \tag{2.22}$$

The parameters p_i fulfil the properties of a probability distribution, i.e. $0 \leq p_i \leq 1$ and $\sum_i p_i = 1$. Therefore, if all the p_i except for one are 0, the

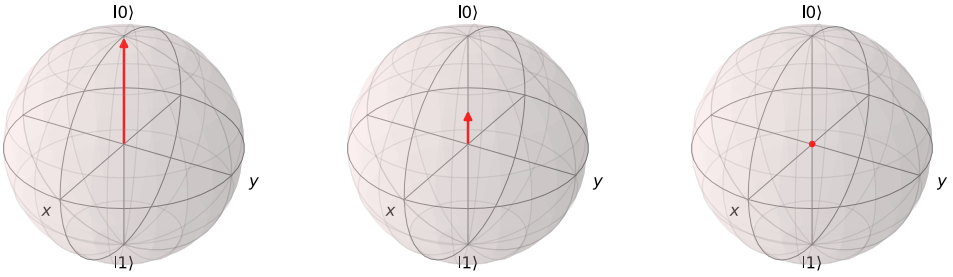
remaining one is 1 and ρ describes a pure state. The density matrix ρ satisfies the properties

- *Hermitian:* $\rho = \rho^\dagger$
- *Positive:* $\rho \geq 0$, such that $\langle\psi|\rho|\psi\rangle \geq 0 \; \forall \, |\psi\rangle \in \mathbb{H}$
- *Unit trace:* $\mathrm{tr}[\rho] = 1$

An additional property following from the above properties of density matrices ρ is that

$$0 < \mathrm{tr}\left[\rho^2\right] \leq \mathrm{tr}\left[\rho\right] = 1. \tag{2.23}$$

Here, for pure states $\mathrm{tr}\left[\rho^2\right] = \mathrm{tr}\left[\rho\right]$, which also holds as a measure known as the *purity*.
One common way to display two-dimensional quantum states (qubits) is by plotting them on the Bloch's sphere, as in Figure 2.1.



(a) $\rho = |0\rangle\langle 0|$ **(b)** $\rho = \frac{2}{3}|0\rangle\langle 0| + \frac{1}{3}|1\rangle\langle 1|$ **(c)** $\rho = \frac{1}{2}|0\rangle\langle 0| + \frac{1}{2}|1\rangle\langle 1|$

Figure 2.1: A pure state (a) is located at the outer hull of the Bloch sphere, while mixed states (b and c) are on the inside of the sphere. A fully mixed state (c) can be found right at the origin. These plots were created using the QuTiP python package [17].

State Evolution of Density Matrices

Similar to quantum states, the Schrödinger equation in Eq. (2.19) can be expressed in terms of density matrices. Computing the time derivative of a density matrix (Eq. (2.22)) shows the equivalence between the Schrödinger equation (2.19) and the *von-Neumann equation*

$$\begin{aligned}
\frac{\mathrm{d}\rho(t)}{\mathrm{d}t} &= \frac{\mathrm{d}}{\mathrm{d}t}\sum_i p_i \, |\psi_i(t)\rangle\langle\psi_i(t)| \\
&= \sum_i p_i \left(\frac{\mathrm{d}\,|\psi_i(t)\rangle}{\mathrm{d}t}\langle\psi_i(t)| + |\psi_i(t)\rangle \frac{\mathrm{d}\,\langle\psi|_i\,(t)}{\mathrm{d}t} \right) \\
&= -i \left(H \sum_i p_i \, |\psi_i(t)\rangle\langle\psi_i(t)| + \sum_i p_i \, |\psi_i(t)\rangle\langle\psi_i(t)| \, H \right) \\
&= -i \left[H, \rho(t) \right].
\end{aligned} \tag{2.24}$$

Here, we plugged in the time-dependent Schrödinger equation and its conjugate transpose in the second line. The von-Neumann equation (Eq. (2.24)) holds as the basis for a further derivation of the dynamics of an open quantum system. By neglecting the environmental degrees of freedom (**DOF**) of the second subspace and taking several assumptions Eq. (2.24) is extended to also describe open system dynamics as we will present in Section 2.1.4.
The formal solution of the von Neumann equation can be expressed in terms of unitary operators similar to in Eq. (2.20) when applied to density matrices

$$\rho(t) = \mathcal{U}\left[\rho(t)\right] = U\rho(0)U^\dagger = e^{-iHt}\rho(0)e^{iHt} \tag{2.25}$$

Here, the transformation on the state $\rho(0)$ is expressed in terms of the quantum map $\mathcal{U}\left[\bullet\right] = U \bullet U^\dagger$.

2.1.2 Quantum Maps

A quantum map (or also quantum channel) $\mathcal{M}$ describes the transformation of a quantum state ρ to another state ρ' such that

$$\rho' = \mathcal{M}\left[\rho\right]. \tag{2.26}$$

These maps are used to describe e.g. unitary evolution as seen in Eq. (2.25), where a quantum state evolves unitarily in time, or other quantum effects like noise or decoherence of the system.

Dynamical maps and composite quantum systems

In a composite quantum state, we use the tensor product ($\otimes$) to combine systems A and B such that

$$\rho_{AB} = \rho_A \otimes \rho_B \in \mathbb{H}_A \otimes \mathbb{H}_B, \tag{2.27}$$

describes the uncorrelated composite state. This state then also evolves unitarily due to its Hamiltonian H_{AB} and when interested in the evolution of A one can trace over the DOF of B to find

$$\rho'_A = \mathcal{E}\left[\rho_A\right] = \mathrm{tr}_B\left(U_{AB}\rho_A \otimes \rho_B U_{AB}^\dagger\right). \tag{2.28}$$

We call $\mathcal{E}$ the dynamical map, which describes how a quantum state ρ_A evolves in time, due to the interaction with its external environment in state ρ_B. It provides a general method to represent quantum processes in open quantum systems. Figure 2.2 illustrates the action of Eq. (2.28).

The dynamical map in Eq. (2.28) is a CPTP map. These maps are formally

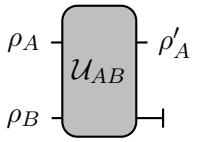


Figure 2.2: The interaction of the composite quantum system describes the evolution of quantum system ρ_A due to its interaction with ρ_B governed by the unitary map $\mathcal{U}_{AB}$.

defined as the following set of linear maps:

$$\text{CPTP} = \{\Lambda : \text{tr}[\Lambda[\rho]] = \text{tr}[\rho] \ \forall\rho \text{ and } (\Lambda \otimes \mathcal{I}_B)[\rho_{AB}] \geq 0 \ \forall\rho_{AB} \geq 0\} \quad (2.29)$$

where $\mathcal{I}_B$ is the identity channel on subsystem B.
The concept of dynamical maps forms a mathematically founded theory of irreversible quantum dynamics that plays an important role in OQS. Here we will deal with a composite quantum system describing the interaction between system S and environment E.
Dynamical maps can also be represented in the Kraus decomposition

$$\rho' = \mathcal{E}[\rho] = \sum_i K_i \rho K_i^\dagger \text{ where } \sum_i K_i^\dagger K_i = \mathbb{1}, \quad (2.30)$$

with the help of the Kraus operators K_i. By their definition, they ensure that ρ' also fulfils the properties of a quantum state in the sense that they represent transformations that map physical states to physical states.
Therefore, it comes as no surprise that the time evolution described by the unitary map (Eq. (2.25)) is also a CPTP map with only one Kraus operator $K_i = U$ that fulfils $K_i^\dagger K_i = U^\dagger U = \mathbb{1}$.
The dynamical map in Eq. (2.28) can also be rewritten in terms of Kraus operators

$$\begin{aligned}
\mathcal{E}[\rho_A] &= \sum_j \langle j|_B \left(U_{AB} \rho_A \otimes \rho_B U_{AB}^\dagger \right) |j\rangle_B \\
&= \sum_j \langle j|_B \left(U_{AB} \rho_A \otimes \sum_i p_i |i\rangle \langle i|_B U_{AB}^\dagger \right) |j\rangle_B \\
&= \sum_{i,j} \sqrt{p_i} \langle j|_B U_{AB} |i\rangle_B \rho_A \sqrt{p_i} \langle i|_B U_{AB}^\dagger |j\rangle_B \\
&= \sum_{i,j} K_{ji} \rho_A K_{ji}^\dagger.
\end{aligned} \quad (2.31)$$

Here, we express the state of subsystem B in its eigenbasis such that $\rho_B = \sum_i p_i |i\rangle \langle i|_B$ and find that $K_{ji} = \sqrt{p_i} \langle j|_B U |i\rangle_B$. By checking $\sum_{ij} K_{ji}^\dagger K_{ji} = \mathbb{1}$

one can see that the dynamical map in Eq. (2.28) is a CPTP map as in Eq. (2.29). Through the Stinespring dilation theorem [18, 19] these two representations are seen as equivalent and from a Kraus form one can always find a non-unique dynamical map describing the transformation.

Fixed Points of Maps

A fixed point ρ^* of a quantum map $\mathcal{M}$ is always mapped onto itself:

$$\mathcal{M}[\rho^*] = \rho^*, \tag{2.32}$$

where once the equilibrium state is reached the system stays in that state.
As an example, any eigenstate $\rho_i = |\psi_i\rangle\langle\psi_i|$ of the Hamiltonian H is a fixed point the unitary map in Eq. (2.25) in a sense that

$$\mathcal{U}[\rho_i] = U\rho_i U^\dagger = e^{-iHt}|\psi_i\rangle\langle\psi_i|e^{iHt} = \underbrace{e^{-iE_it}e^{iE_it}}_{=1}|\psi_i\rangle\langle\psi_i| = \rho_i, \tag{2.33}$$

Here we used that the eigenvalue equation (2.14) also holds for analytical functions f (see Eq. (2.8)), e.g. $f(H) = e^{iHt}$.
Fixed points represent stable states of a quantum system under evolution and are therefore particularly important. These processes are an important part of this work and we will see that an equilibrium state is a fixed point of a thermodynamic dynamical map.

2.1.3 Fundamentals of OQS

Any realistic model used to represent observed physical phenomena cannot be considered closed since no system is ever completely isolated from its environment [20]. Every energy loss in the system has to be taken into account by its environment. In a closed system, there is no mechanism in place to account for these losses. An important result of this exchange is dissipative behaviour, which is an effect, that the framework of OQS is perfectly capable of describing.
When dealing with open systems composed of a system S embedded in a larger system, called environment E, the framework of open quantum systems becomes essential to faithfully describe the dynamic evolution of the open system.

Open Quantum System Setup

Mathematically speaking the open system S is embedded in an environment E with which it interacts. The interaction takes place in a composite Hilbert

space $\mathbb{H}_S \otimes \mathbb{H}_E$.
The energy levels of an open quantum system are typically described in terms of three main components which are illustrated in Figure 2.3:

- **System Hamiltonian H_S:** is the free Hamiltonian of the system, describing the energy of the system and influences the system dynamics
- **Environment Hamiltonian H_E:** is the free Hamiltonian of the environment, representative of the energy of the environment that due to its interaction with the system also influences the system dynamics.
- **Interaction Hamiltonian H_{SE}:** this Hamiltonian determines how exactly the system and environment interact with one another.

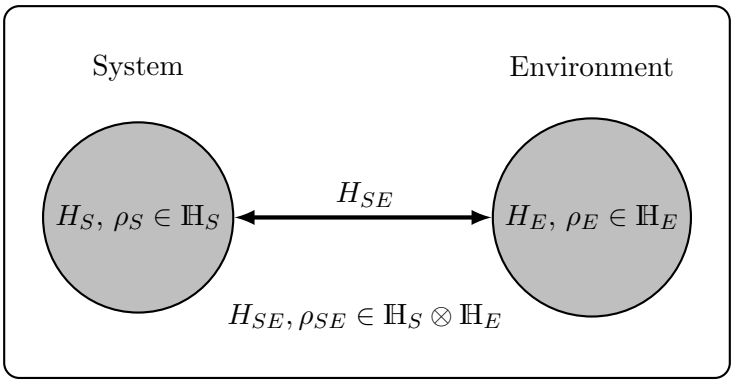


Figure 2.3: Schematic diagram of an open quantum system S in contact with an environment E . The system interacts with the environment and the interaction Hamiltonian H_{SE} governs this interaction.

This set of Hamiltonians forms the total Hamiltonian of the open quantum system

$$H = H_S + H_E + H_{SE}. \tag{2.34}$$

Here one has to consider that the system and environment's free Hamiltonians are each defined with respect to their subspaces $\mathbb{H}_S$ and $\mathbb{H}_E$. Therefore the sum of these Hamiltonians has to be understood such that $H_S + H_E \equiv H_S \otimes \mathbb{1}_E + \mathbb{1}_S \otimes H_E$. The interaction Hamiltonian H_{SE} acts on both subspaces and can be represented in the respective composite basis

$$H_{SE} = g \sum_{i,j,\mu,\nu} c_{i\mu j\nu} \left|i\right\rangle \left\langle j\right|_S \otimes \left|\mu\right\rangle \left\langle \nu\right|_E . \tag{2.35}$$

Here, basis elements of the system are denoted by lowercase Latin letters and in the environment basis by lowercase Greek letters. For future reference

we will require that subscripts S and E are considered with respect to each individual subspace, such that $|i\rangle \equiv |i\rangle_S$ and $|\mu\rangle \equiv |\mu\rangle_E$.
The coefficient g in Eq. (2.35) is a real-valued scaling factor, that we will use later when finding a description of the open system dynamics.
Since the interaction Hamiltonian H_{SE} is a Hermitian operator we can restrict its components $c_{i\mu j\nu}$ in a chosen joint system-environment basis, such that by demanding

$$H_{SE} = g \sum_{i,j,\mu,\nu} c_{i\mu j\nu} |i\rangle \langle j| \otimes |\mu\rangle \langle \nu| = g \sum_{i,j,\mu,\nu} c^*_{j\nu i\mu} |i\rangle \langle j| \otimes |\mu\rangle \langle \nu| = H^\dagger_{SE} \quad (2.36)$$

we find that

$$c_{i\mu j\nu} = c^*_{j\nu i\mu}. \quad (2.37)$$

Markovianty in classical systems
Markovianity is an assumption that holds for many physically relevant scenarios. Classical Markovian systems are those, where the future evolution of a system only depends on its present state and not on any further in the past. The state evolution of a classical process $\{X_t\}$ can be described in terms of probabilities, where X_t are random variables describing the outcome of a random process, e.g. a coin toss. Here the probability distributions of any future state X_{t+1} depend only on the current state X_t and not on the states that came before. A classical process is said to be Markovian if it fulfils the Markov condition

$$P\left(X_{t+1}|X_t, X_{t-1}, \ldots X_0\right) = P\left(X_{t+1}|X_t\right). \quad (2.38)$$

Markovianty in quantum systems
As an analogy in closed quantum systems, the Schrödinger equation (Eq. (2.19)) and also the von-Neumann equation (Eq. (2.24)) are Markovian, since the evolved state only depends on the current state. In open quantum systems where an environment is present, this simple structure is potentially not true any more, since past interactions with the environment might influence future dynamics. Markovian master equations hold as a 'middle ground', that keeps the dynamics memoryless by describing them with a differential equation that only depends on the current state of the system, while still incorporating interactions with the environment. The memoryless nature of Markovian systems is often understood in terms of rapidly vanishing memory effects in the environment. In that sense, the environment is not unaffected by the interaction it had with the system but forgets about them very fast. This fundamental concept plays a major role in describing the dynamics of a system and will

be exhibited from different angles when we introduce various paths to find a quantum master equation. In the next section we will introduce the quantum semigroup property, which can be seen as the formal definition of Markovianity in OQS.

2.1.4 Quantum Master Equations

Quantum master equations are a tool to describe the dynamics of an open quantum system. In their easiest application, on Markovian dynamics, they yield a simplified description of the system dynamics, by applying several approximations to an initially unitary evolution of the composite $S - E$ state. Their solution is the description of the irreversible time evolution of the system state governed by its interaction with the environment. Therefore, they describe the dynamics of a system that interacts with an environment. But first we will give an intuitive example of how to derive such an ME in a classical setup.

Statistical (classical) master equation

Initially, master equations were introduced to describe the time evolution of probabilistic systems on the hand of differential equations. These equations are suitable for describing, among others, decay processes [6]. Based on an example from Ref. [21] we highlight how a probabilistic master equation can be found and in Section 2.3.3 we show that in the infinite time limit the dynamic evolution leads to an equilibrium state.

Consider a two-level system, with a ground and an excited state, referred to as $|g\rangle$ and $|e\rangle$. Here $P_g(t)$ and $P_e(t)$ denote the probabilities of the system being found in the ground or excited state at time t and they fulfil $P_g(t) + P_e(t) = 1$. The decay $|e\rangle \to |g\rangle$ and excitation processes $|g\rangle \to |e\rangle$ can then be described by considering the probabilities for the next time step $t + \Delta t$. By invoking that the state only depends on the previous one and not the entire history of the state we already assume that the system is Markovian in the sense of classical probability theory (c.f. Eq. (2.38)). The probability of the ground state population

$$P_g(t + \Delta t) = P_g(t)(1 - \gamma(e \to g))\Delta t + P_e(t)\gamma(g \to e)\Delta t + \mathcal{O}(\Delta t^2), \quad (2.39)$$

is expressed in terms of the transition rates γ. Here $1 - \gamma(e \to g)\Delta t$ is the probability of the system staying in the ground state and $\gamma(g \to e)\Delta t$ is the probability for the system jumping from the ground to the excited state during time Δt. We disregard terms of $\mathcal{O}(\Delta t^2)$, since we are later going to take the limit of infinitesimal time steps ($\Delta t \to 0$), where these terms are outweighed

by terms of $\mathcal{O}(\Delta t)$. Disregarding terms of order $\mathcal{O}(\Delta t^2)$ excludes excitations followed by a de-excitation back to the ground state within one time step Δt and other unlikely events of even higher order.
Rearranging Eq. (2.39) to compute the change in the probability with $\Delta P_g(t) = P_g(t+\Delta t) - P_g(t)$ and dividing by Δt allows us to express the change rate of the probability in the continuous-time limit as $\Delta t \to 0$ and we find

$$\frac{\mathrm{d}P_g(t)}{\mathrm{d}t} = -\gamma(g \to e)P_g(t) + \gamma(e \to g)P_e(t). \tag{2.40}$$

By setting up an equation similar to Eq. (2.39) for the probability of the system being in the excited state, we find its change rate

$$\frac{\mathrm{d}P_e(t)}{\mathrm{d}t} = -\gamma(e \to g)P_e(t) + \gamma(g \to e)P_g(t). \tag{2.41}$$

This system of first-order differential equations (Eqs. (2.40) and (2.41)) forms a master equation describing the time evolution of the probabilities of the system being in either the ground or the excited state. This master equation can be solved analytically to the time evolution of the probability distribution

$$\begin{aligned} P_g(t) &= P_g(t_0)\gamma(e \to g) - P_e(t_0)\exp\left\{-\left(\gamma(e \to g) + \gamma(g \to g)\right)(t - t_0)\right\} \\ P_e(t) &= P_g(t_0)\gamma(g \to e) + P_e(t_0)\exp\left\{-\left(\gamma(e \to g) + \gamma(g \to g)\right)(t - t_0)\right\}. \end{aligned} \tag{2.42}$$

In the course of this work we will use quantum master equations, to study the time evolution of density matrices ρ instead of probability distributions P and start by introducing the formal definition of Markovianity in OQS, which is deeply linked to a Markovian quantum master equation.

Quantum master equations and the semigroup property

The time evolution of an open quantum system, that is initially uncorrelated to its environment, can be expressed in terms of a dynamical map $\mathcal{E}$ similar to Eq. (2.28). It describes the system evolution by a unitary transformation of the composite system and afterwards taking the partial trace over the environment's DOF. The time-dependent state $\rho(t)$ in a time-independent environment is given by the dynamical map

$$\rho_S(t) = \Lambda_t\left[\rho_S(0)\right] = \mathrm{tr}_E\left(U(t,0)\ \rho_S(0) \otimes \rho_E\ U^\dagger(t,0)\right). \tag{2.43}$$

It is reasonable to assume that a quantum system is Markovian if the characteristic time scales in which the environment correlations decay are much

faster than the time scales of the system. Dynamical maps that fulfil

$$\Lambda_t = \Lambda_{t-s} \circ \Lambda_s \ \forall \ t \geq s \geq 0 \text{ and } \lim_{t \to 0^+} \Lambda_t = \mathcal{I} \tag{2.44}$$

are said to fulfil the semigroup property, which is seen as the formal definition of Markovianity in open quantum systems.
It fulfils the properties of a mathematical group in that it is associative $\Lambda_t = \Lambda_{t-s} \circ \Lambda_s$ and the identity element is defined as t approaches 0 by $\Lambda_0 = \mathcal{I}$. However, there does not exist an inverse element Λ_{-t} such that $\Lambda_t \circ \Lambda_{-t} = \mathcal{I}$. Hence, it is called a semigroup instead of a group and one cannot reconstruct the history of a system through the semigroup map Λ_t since $t \geq 0$. The map only determines how the state evolves into the future based on its current state.
Time evolution in Markovian open quantum systems is a fundamentally different description than that of unitary evolution describing the dynamics in closed quantum systems, where time evolution in both directions is possible.
For all systems where the semigroup property holds, it is possible to state the time evolution in terms of a linear map $\mathcal{L}$, the generator of the semigroup. It can be shown [7] that the map Λ_t can then be expressed in terms of its semigroup generator

$$\Lambda_t[\bullet] = e^{\mathcal{L}t}[\bullet]\,. \tag{2.45}$$

Eq. (2.45) is the formal solution to a first-order differential equation

$$\frac{\mathrm{d}\rho(t)}{\mathrm{d}t} = \mathcal{L}[\rho(t)]\,, \tag{2.46}$$

which is called the Markovian quantum master equation. Eq. (2.46) leads to the most general form of a Markovian quantum master equation. We will now present a sketch of a microscopic approach to find the structure of this Markovian ME.

The Markovian quantum master equation

This section sketches the outline of the derivation of a Markovian quantum master equation in a microscopic approach as presented in Section 3.3 of [7]. It employs several assumptions referred to as the Born-Markov approximation, which are summarized here.
This approach starts with a description of the total system ρ_{SE} dynamics as given by its total Hamiltonian H in Eq. (2.34). The interaction between the system and the environment is represented by the interaction Hamiltonian H_{SE} and the isolated evolution of the subsystems by their free Hamiltonians

H_S and H_E. The unitary evolution of this composite quantum system can be described by the von Neumann equation given in Eq. (2.24). Finding the dynamics of the open quantum system S is achieved by taking the partial trace over the environment's DOF and making several assumptions commonly referred to as Born Markov assumptions [7].
After applying these approximations one can find a Markovian quantum master equation in Gorini-Kossakowski-Sudarshan-Lindblad (**GKSL**) form

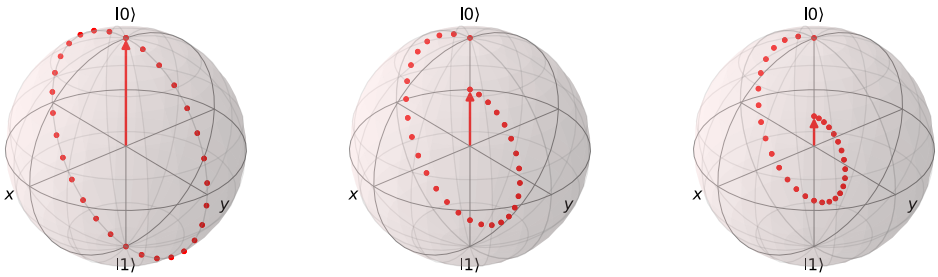
$$\mathcal{L}\left[\rho_S\right] = \frac{\mathrm{d}\rho_S}{\mathrm{d}t} = -i\underbrace{\left[H_S', \rho_S\right]}_{\mathcal{H}[\rho_S]} + \underbrace{\sum_{i,j}\left(L_{ij}\rho_S L_{ij}^\dagger - \frac{1}{2}\left\{L_{ij}^\dagger L_{ij}, \rho_S\right\}\right)}_{\mathcal{D}[\rho_S]}. \tag{2.47}$$

The so-called, Lindbladian $\mathcal{L}$ defines a generator of a quantum dynamical semigroup in its most general form. The first part $\mathcal{H}$ describes the unitary evolution of the system governed by the system's Hamiltonian $H_S' = H_S + H_{LS}$, rescaled by the Lamb shift term H_{LS}. This contribution renormalizes the system's energy levels due to its interaction with the environment [7, 22, 23]. The second part $\mathcal{D}$ describes the dissipative evolution of the system due to its interaction with the environment governed by the so-called Lindblad jump operators L_{ij}.
The GKSL equation is usually solved numerically and allows for an investigation of general features like irreversibility, and relaxation to equilibrium [7].
In Figure 2.4 we illustrated the numerical solutions of the time evolution of an open quantum system. Here, one can see how the initially pure state $\rho(0)$ loses its purity due to the interaction with the environment. It becomes ever more mixed over time and with increasing interaction strength Γ, it approaches an equilibrium state with its environment ever faster.

In the following section, we will present a way to derive a Markovian quantum master equation based on a simple collision model. This will allow us to keep track of all contributions to the dynamic description and therefore, gain a deeper understanding of all the contributing factors to the open quantum system dynamics.

2.2 Markovian Collision Models

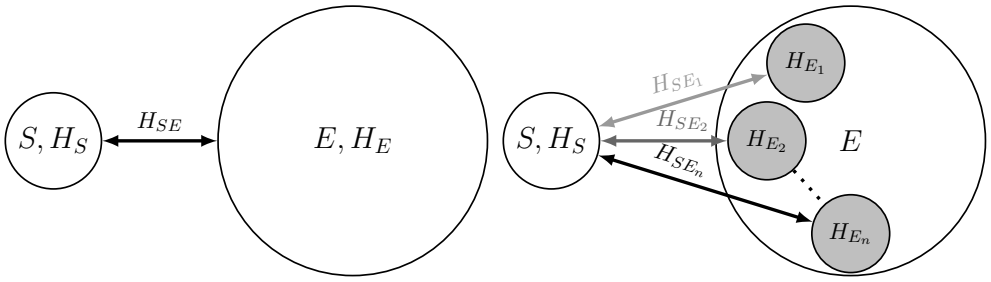
Similar to the microscopic approach presented in Subsection 2.1.4, a collision model can be used to describe the interaction of a System S with its environment E. In the basic version of this model [8, 15, 24–28] the dynamics



(a) $\Gamma = 0$ **(b)** $\Gamma = 0.1$ **(c)** $\Gamma = 0.2$

Figure 2.4: Time evolution of the initial state $\rho_S(0) = |0\rangle\langle 0|$ with its free Hamiltonian $H'_S = \sigma_x$, due to the open system dynamics following from the Lindblad jump operators of the form $L_{ij} = \sqrt{\Gamma}\sigma_x$ plotted on the Bloch sphere. The dynamic evolution is illustrated on the hand of three different dampening factors Γ and shows how an initially pure state loses its purity in 30 time steps for $t \in [0, \pi]$. Each time step is represented by a red dot, while the final state is represented by a red vector. Created using the QuTip python package [17]

are modelled such that S is in contact with individual parts E_i of the environment consecutively. The environment is assumed to be described by a bath comprised of a large number of particles. These particles, also referred to as ancillas, are considered non-interacting with each other in a Markovian collision model (**CM**). The design of the environment differs vastly from the microscopic description, where the system is coupled to all environmental modes at once instead of interacting with them individually in a CM as illustrated in Figure 2.5.



(a) microscopic approach **(b)** collision model

Figure 2.5: In the microscopic approach (a), the system S interacts with all modes of the environment E at the same time. In a collision model (b) the system S interacts with each ancilla E_i consecutively. The consecutive nature of the interaction is illustrated by the fading grey colour tone of the arrows of interactions further down in the past.

The open system evolution is initially described in an inherently discrete manner. This follows from the nature of a collision model where successive pairwise

interactions between S and E occur. Only one interaction between S and E happens at a time and in Markovian CMs each environmental ancilla is excluded from any further interaction with S afterwards. Each of these collisions is modelled by a dynamical map, similar to Eq. (2.28).
To get a continuous description of the open system dynamics one takes the continuous time limit, which yields a Markovian master equation of GKSL form [24, 29].

2.2.1 Setup of a Markovian Collision Model

For the setup of the collision model, we follow the approach of Ciccarello [16]. Alternative approaches are presented in the reviews and tutorials [30, 31] or in a mathematical rigours form in the work of Altamirano et al. [32].
The collision model describes the evolution of an open quantum system. Therefore, its dynamics are based on interactions between S and E. As depicted in Figure 2.5, the environment is modelled by each ancilla's individual Hamiltonian H_{E_n} and its interaction with S is governed by a time-independent Hamiltonian H_{SE_n}. In this approach, the bath is comprised of identical states η with identical energies, i.e. $H_{E_n} \equiv H_E$, where all the subspaces that the operator acts trivially on are omitted.
Each individual interaction is modelled by an initially unitary interaction of the composite quantum system

$$\mathcal{U}_n [\bullet] = U_n \bullet U_n^\dagger = e^{-iH_n \Delta t} \bullet e^{iH_n \Delta t} \tag{2.48}$$

for the time step length Δt and the total Hamiltonian H_n, defined similar to the one used for the general open quantum system approach in Eq. (2.34). However, due to the nature of consecutive interactions it is defined for each environmental ancilla E_n individually by

$$H_n = H_S + H_{E_n} + H_{SE_n}. \tag{2.49}$$

It is to be noted here that the respective Hilbert spaces of S and E_n can be of any dimension and that the subspaces that are acted on trivially are omitted. From now on and throughout the rest of this thesis $\rho \equiv \rho_S$ is always the state representing the system DOF and $\eta \equiv \eta_E$ the environment's. The state of the composite system and environment is represented by $\sigma \equiv \sigma_{SE}$.
The aim is to describe the system dynamics with a model as depicted in Figure 2.6. Here ρ_0 represents the system state before any interaction with

the environmental ancillas η. At this point, S is uncorrelated with all the ancillas and the joint S-E state is given by the product state

$$\sigma_0 = \rho_0 \otimes \eta \otimes \cdots \otimes \eta \tag{2.50}$$

The state of the joint system after the n-th interaction is then given by applying the unitary map in Eq. (2.48) consecutively on the initial state σ_0, which leads to the evolved state

$$\sigma_n = \mathcal{U}_n \left[\ldots \mathcal{U}_1 \left[\sigma_0 \right] \right]. \tag{2.51}$$

Taking the partial trace over the environmental DOFs then leads to the final system state ρ_n.
Assuming that each environment state is excluded from any further interaction and that there are no ancilla-ancilla interactions ensures that fresh ancilla states are uncorrelated with the system. Therefore, the system state always interacts with η, which allows for expressing individual interactions in the form of a dynamical map $\mathcal{E}$ acting on the previous system state ρ_{n-1} to find the evolved state

$$\rho_n = \mathcal{E}\left[\rho_{n-1}\right] = \mathrm{tr}_{E_n}\left(U_n \ \rho_{n-1} \otimes \eta \ U_n^\dagger\right). \tag{2.52}$$

Figure 2.6 illustrates the discrete nature of the interaction based on the unitary interaction between S and each individual environment ancilla E_i. By applying the dynamical map in Eq. (2.52) we take the partial trace over the environmental DOF after the unitary interaction. Modelling the interaction like this makes any ancilla-ancilla correlations impossible and the systems state is only correlated with the past environment states and never with the ones it hasn't interacted with yet.

Through consecutive evolution by applying the CPTP map $\mathcal{E}$ n-times to the initial state ρ_0 in equal time steps Δt we find

$$\rho_n = \mathcal{E}^n\left[\rho_0\right]. \tag{2.53}$$

The open dynamics of S from state ρ_n to $\rho_{n'}$ (i.e. $n' > n$) depends only on the state of S at step n. The system, therefore keeps no memory of its past and the evolution to the next state only depends on the system's current state, making this CM Markovian by construction.
The dynamical map $\mathcal{E}$, therefore fulfils the properties of a semigroup and by referring to $\mathcal{E}^n = \Lambda_n$ we define it as in Eq. (2.44). The Markovian properties hint that in the continuous-time limit, we will then find a Markovian master

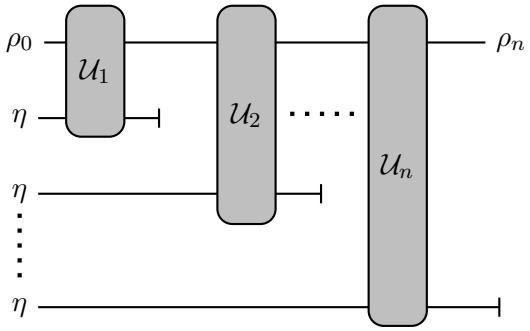


Figure 2.6: A simple collision model where the initial system input state ρ_0 interacts with environment states η consecutively. Each interaction is considered acting on its respective subspace $\mathbb{H}_{E_i}$, represented by a unitary interaction $\mathcal{U}_i$. The environment degrees of freedom are traced out after each interaction.

equation of GKSL form.

2.2.2 Discrete Master Equation from a Markovian Collision Model

Appling the unitary map in Eq.(2.48) to the joint S-E state can be approximated by a second order series expansion

$$U_n = e^{-iH_n\Delta t} = \mathbb{1} - i\Delta t H_n - \frac{(\Delta t)^2 H_n^2}{2} + \mathcal{O}(\Delta t^3). \tag{2.54}$$

We require the time steps Δt to be small enough such that terms of order $\mathcal{O}(\Delta t^3)$ vanish. Computing the difference of the evolution in one time step $\Delta\rho_n = \mathcal{E}[\rho_n] - \rho_n$ using the definition of the discrete dynamical map $\mathcal{E}$ in Eq. (2.52) we find

$$\begin{aligned}\Delta\rho_n = &-i\Delta t\left([H_S,\rho_n] + \mathrm{tr}_E\left[H_{SE_n},(\rho_n\otimes\eta)\right]\right) - \\ &- (\Delta t)^2\ \mathrm{tr}_{E_n}\Bigg(\frac{1}{2}\left\{(\tilde{H}_n^2 + 2\tilde{H}_n H_{SE_n} + H_{SE_n}^2),(\rho_n\otimes\eta)\right\} + \\ &+ \tilde{H}_n(\rho_n\otimes\eta)\tilde{H}_n + H_{SE_n}(\rho_n\otimes\eta)\tilde{H}_n + \tilde{H}_n(\rho_n\otimes\eta)H_{SE_n} + \\ &+ H_{SE_n}(\rho_n\otimes\eta)H_{SE_n}\Bigg) + \mathcal{O}(\Delta t^3).\end{aligned} \tag{2.55}$$

Here, we collected the free Hamiltonians of system and environment to $\tilde{H}_n \equiv H_S + H_{E_n}$. To further simplify this expression we scale the Hamiltonians, such that

$$H_S, H_{E_n} = \mathcal{O}(\omega) \qquad H_{SE_n} = gV_n = \mathcal{O}(g) \qquad \omega \ll g. \tag{2.56}$$

Here, the coefficient g is the interaction strength multiplied by the unscaled interaction Hamiltonian V_n. $\tilde{H}_n$ is also of order $\mathcal{O}(\omega)$, which is very small when compared with the scaling g of the interaction Hamiltonian. We used this to eliminate the $\tilde{H}_n$ when they are multiplied with Δt, while terms of order $g\Delta t$ are finite in the continuous-time limit. Terms of order $\omega g\Delta t$ will vanish in this limit. Each of these terms in Eq. (2.55) can then be evaluated to either vanish because they are very small when compared to the coefficient g or by simply using the linearity of the partial trace.
To summarize, we demand for the coefficients ω and g in the continuous time limit that while $g^2\Delta t$ is finite,

$$g\omega\Delta t \to 0,\ \omega\Delta t \to 0,\ \omega^2\Delta t \to 0, \tag{2.57}$$

as $\Delta t \to 0$. These terms then do not contribute to the overall system dynamics, since their effect is very small when compared to the other terms. Therefore, it is implied that the product of g with a value $x = 0$ vanishes, such that

$$\lim_{g\to\infty} gx = 0\ \forall x = 0. \tag{2.58}$$

This condition is necessary to be able to get finite results of the commutator of the free Hamiltonians together with $H_{SE_n} = gV_n$ in Section 3.7.
Collecting all the remaining terms leads to the discrete-time master equation

$$\begin{aligned}\frac{\Delta\rho_n}{\Delta t} &= -i\left[H_S + g\mathrm{tr}_{E_n}\left(V_n\eta\right), \rho_n\right] + \\ &\quad + g^2\Delta t\left(\mathrm{tr}_{E_n}\left(V_n\rho_n\otimes\eta V_n\right) - \frac{1}{2}\left\{\mathrm{tr}_{E_n}(V_n^2\eta), \rho_n\right\}\right),\end{aligned} \tag{2.59}$$

by additionally dividing Eq. (2.55) by Δt.
To express this master equation in terms of Lindblad jump operators $L_{\nu\gamma}$, the rearrangement

$$\begin{aligned}\mathrm{tr}_{E_n}\left(V_n\rho_n\otimes\eta V_n\right) &= \sum_\nu \langle\nu| V_n\rho_n\otimes\left(\sum_\gamma p_\gamma |\gamma\rangle\langle\gamma|\right) V_n|\nu\rangle \\ &= \sum_{\gamma,\nu}\sqrt{p_\gamma}\langle\nu| V_n|\gamma\rangle\rho_n\sqrt{p_\gamma}\langle\gamma| V_n|\nu\rangle = \sum_{\gamma,\nu} L_{\nu\gamma}\rho_n L_{\nu\gamma}^\dagger.\end{aligned} \tag{2.60}$$

in the eigenbasis of S and E_n suffices. Here, we expressed η in terms of its eigenbasis and used the fact that the system state ρ_n commutes trivially with eigenstates of the environment subsystem. The final result follows from the

definition

$$L_{\nu\gamma} := \sqrt{p_\gamma} \langle \nu | V_n | \gamma \rangle . \tag{2.61}$$

With the help of the Lindblad jump operators in Eq. (2.61), the term within the anti-commutator of Eq. (2.59) can be rewritten as

$$\begin{aligned} \mathrm{tr}_{E_n}(V_n^2 \eta) &= \sum_{\mu,\gamma} \langle \mu | V_n^2 p_\gamma | \gamma \rangle \langle \gamma | \mu \rangle \\ &= \sum_{\gamma,\nu} \sqrt{p_\gamma} \langle \gamma | V_n | \nu \rangle \sqrt{p_\gamma} \langle \nu | V_n | \gamma \rangle = \sum_{\gamma,\nu} L_{\nu\gamma}^\dagger L_{\nu\gamma}. \end{aligned} \tag{2.62}$$

Due to the discrete nature of the CM, the found master equation in Eq. (2.59) is based on differentials of discrete time steps Δt. To get a continuous-time master equation we will take the continuous-time limit in the next section, allowing us to express the master equation as a first-order differential equation.

2.2.3 Continuous Time Master Equation

We want to describe the evolution of the system state ρ up until time t. Since this happens in time steps Δt we find after a total number of steps N that $t = N\Delta t$. Or, equivalently a relation for the time step length

$$\Delta t = \frac{t}{N}. \tag{2.63}$$

For an infinite number of steps, i.e. $N \to \infty$, follows that $\Delta t \to 0$. If g is chosen to be a finite constant, the dissipator in Eq. (2.59) vanishes. This vanishing dissipative behaviour is discussed in detail in [32, 33]. Therefore we need to carefully scale g together with $\Delta t \to 0$ such that the newly introduced constant

$$\Gamma = g^2 \Delta t \text{ for } \Delta t \to 0,\ g \to \infty, \tag{2.64}$$

is finite.

However, g also appears in the unitary part of Eq. (2.59) without being scaled by Δt. This, so called, Lamb shift term $H_{LS} = g\mathrm{tr}_{E_n}(V_n \eta)$ therefore diverges in the limit of $g \to \infty$. It is often assumed that the average of this term is zero or that it can be renormalized by incorporating it with the system Hamiltonian H_S [16, 30]. The divergent behaviour of H_{LS} will further be discussed in Section 4.2.1, where we also present alternative approaches.

By applying Eq. (2.64) to Eq. (2.47) we then find a continuous time master equation of GKSL form

$$\frac{\mathrm{d}\rho}{\mathrm{d}t} = -i\left[H_S + H_{LS}, \rho\right] + \Gamma \sum_{\nu\mu} \left(L_{\nu\mu} \rho L_{\nu\mu}^\dagger - \frac{1}{2} \left\{ L_{\nu\mu}^\dagger L_{\nu\mu}, \rho \right\} \right). \tag{2.65}$$

The system state ρ in Eq. (2.65) is time-dependent and we imply that $\rho \equiv \rho(t)$. The same dynamics are described by plugging in the $L_{\mu\nu}$ as given in Eq. (2.61) again and finding a continuous time evolution in terms of the Hamiltonians. For the sake of simplicity, we will from now drop the index of all Hamiltonians that act on the n-th subsystem since we assume that the system interacts with identical ancillas in each collision. Therefore, from now on

$$H_{SE_n} \equiv H_{SE} = gV \qquad H_{E_n} \equiv H_E. \tag{2.66}$$

Since the Markovian collision model approach also exhibits the semigroup property (Eq. (2.44)) we will refer to the resulting Lindbladian

$$\mathcal{L}[\rho] = \frac{\mathrm{d}\rho}{\mathrm{d}t} = -i[H_S + H_{LS}, \rho] + \Gamma\left(\mathrm{tr}_E(V\rho\eta V) - \frac{1}{2}\left\{\mathrm{tr}_E(V^2\eta), \rho\right\}\right) \tag{2.67}$$

as the generator of the semigroup map

$$\Lambda_t[\rho] = e^{\mathcal{L}t}[\rho]. \tag{2.68}$$

The found generator in Eq. (2.67) follows the general structure of the Lindbladian $\mathcal{L} = -i\mathcal{H} + \mathcal{D}$ of a GKSL master equation. As in the result from the microscopic derivation in Section 2.1.4, the unitary part $\mathcal{H} = \mathcal{H}_S + \mathcal{H}_{LS}$ is rescaled by the Lamb shift Hamiltonian H_{LS} and from Eq. (2.59) we can read off that the energy shift of the unperturbed system Hamiltonian is precisely

$$\mathcal{H}_S[\rho] = [H_S, \rho], \tag{2.69}$$

while the Lamb shift is defined by

$$\mathcal{H}_{LS}[\rho] = [H_{LS}, \rho] = [\mathrm{tr}_E(H_{SE}\tau), \rho]. \tag{2.70}$$

On the other hand, the dissipator $\mathcal{D}$ is scaled by the finite constant Γ and since Eq. (2.59) and Eq. (2.67) are equivalent it reads

$$\begin{aligned}\mathcal{D}[\rho] =& \Gamma\sum_{\nu\mu}\left(L_{\nu\mu}\rho L_{\nu\mu}^\dagger - \frac{1}{2}\left\{L_{\nu\mu}^\dagger L_{\nu\mu}, \rho\right\}\right)\\ =& \Gamma\left(\mathrm{tr}_E(V\rho\otimes\tau V) - \frac{1}{2}\left\{\mathrm{tr}_E(V^2\tau), \rho\right\}\right)\end{aligned} \tag{2.71}$$

Even though the assumptions in the microscopic approach differ vastly from the collision model introduced here, they both yield a GKSL equation. Ref. [31] compares the assumptions taken in both approaches and by that highlights

another benefit of the collision model: no further assumptions need to be taken once the model is set up and the continuous time limit is taken. In the collision model, there is no need to take the Born-Markov approximation since it is already implied by the setup of the collision model, by Eqs. (2.50) and the Markovian nature of the chosen collision model in Figure 2.6 by tracing over each ancilla's DOF and excluding it from any further interaction with S and therefore not allowing for any ancilla-ancilla collisions.
Taking account of effects like ancilla-ancilla is done by an extension of a CM. These CMs are referred to as non-Markovian. A few examples of how the formalism of collision models might be extended are presented in an outlook in Section 5.2.

2.3 Quantum Thermodynamics

In this section, we will equip the before-found collision model setup with thermodynamic assumptions such that it results in a thermodynamic GKSL equation.
Classical thermodynamics is a theory that allows one to describe otherwise complex systems comprised of a large number of particles in equilibrium states by only a few macroscopic parameters. This theory is formulated based on a few postulates justified by experimental observations. These postulates ultimately allow for the formulation of the laws of thermodynamics and fundamental relations that fully describe the properties of thermodynamic equilibrium states.
Thermodynamics, therefore is a macroscopic theory, that describes the state of a system with only a few parameters instead of trying to describe the dynamics of each individual particle within an enclosed space. This approach is possible since thermodynamic experiments are slow and coarse-grained when compared to an atomic scale. This simplification can be traced back to statistical properties and is made possible because these systems are so large and not despite that. Extending this thermodynamic framework to small systems and also to study non-equilibrium systems gave rise to the advent of quantum thermodynamics, summarized in review papers [5, 34].
Thermodynamic systems are known to equilibrate in a classical setting and since quantum systems reproduce the laws of classical thermodynamics in the thermodynamic limit we expect that these thermodynamic principles can also be applied to open quantum systems. In this thesis we want to examine the path towards equilibrium for quantum processes by applying thermodynamic assumptions to these open systems.

2.3.1 Energy Conservation

Energy conservation is the foundation of many physical theories. In classical thermodynamics energy conservation is postulated and manifests the first law of thermodynamics. In a dissipative system, energy is lost to the environment. Therefore, in open quantum systems, that exchange energy with their environment, energy within the system itself is not necessarily conserved. However, the concept of strict energy conservation (**SEC**) [35], states that every energy change in S has to be met in E. This condition is formulated in terms of the Hamiltonians in Eq. (2.34) as the commutation relation

$$[H_{SE}, H_S + H_E] = 0. \tag{2.72}$$

In Appendix C.1 we illustrated how this commutation relation restricts the eigenenergies of an open quantum system. It then becomes clear that due to SEC every energy change in S has to be met in E and therefore, no energy is lost in between them.

2.3.2 Entropy Maximization

Postulating that thermodynamic systems assume the state for which the entropy is maximized is fundamental for formulating the second law of thermodynamics. A consequence thereof is that these systems monotonically approach the steady state. After the steady state is reached, the system doesn't change in time and it can be described by its intrinsic properties and there is no need to take account of how the system reached its steady state. When describing a system with a quantum map, a fixed point of the map constitutes a steady state.
In quantum thermodynamics, there exists a unique state that maximizes the von Neumann entropy

$$S = -k_B \mathrm{tr}\rho \log \rho \tag{2.73}$$

for fixed energy $\langle H \rangle = \mathrm{tr}(H\rho)$. It is a thermal equilibrium state defined as

$$\rho_{th} \equiv \frac{e^{-\beta H_S}}{\mathrm{tr}\left(e^{-\beta H_S}\right)}, \text{ where } \beta \equiv \frac{1}{k_B T} \tag{2.74}$$

and is referred to as either *thermal* or *Gibbs state* since it can be seen as the quantum version of the canonical (Gibbs) ensemble known from statistical mechanics. Thermal states are completely passive, which means that no energy can be extracted unitarily [36, 37].

Here β is the inverse temperature, where we will set the Boltzmann constant $k_B = 1$ as we are working in natural units throughout this thesis.
As we will shortly see, the thermal state's equilibrium properties will also play a role in the dynamic evolution of the system in that it will turn out as the fixed point of a thermodynamic dynamical map.

2.3.3 Thermal Equilibrium and Thermalization

In open quantum systems equilibration is considered a process where the system approaches its steady state. After reaching this fixed point the states before cannot be recovered by the map that led to the equilibrium condition [38].
Usually, systems reach equilibrium after a very long time. We want to illustrate this behaviour on hand of the example of the classical master equation in Section 2.1.4. Considering the limit $t \to \infty$ in Eq. (2.42) shows that the probability distributions converge towards a time-independent equilibrium state and can be described by the ratio

$$\frac{P_g^{eq}}{P_e^{eq}} = \frac{\gamma(e \to g)}{\gamma(g \to e)}. \tag{2.75}$$

This result shows that for a higher transition rate from $|e\rangle \to |g\rangle$ a population in the ground state becomes more likely in the time-independent probability distribution at equilibrium conditions. Eq. (2.75) is a general property that holds in closed, isolated, finite physical systems called a detailed balance (**DB**) condition [39]. Detailed balance conditions have also been found for open quantum systems and can be identified with thermal equilibrium [4, 40]. Detailed balance is so closely related to equilibrium that, the violation of a DB conditions has been employed as an indicator for out-of-equilibrium conditions [41, 42]. In the next section we will find a master equation following from a thermodynamic collision model, that we will ultimately apply to its steady state to find a detailed balance condition describing thermal equilibrium in Section 3.6.1.

2.4 Thermodynamic Master Equation

Applying the thermodynamic considerations of Section 2.3 to the Markovian collision model derived in Section 2.2 implies certain restrictions on the master equation of GKSL form in Eq. (2.65). Compatibility of open quantum system dynamics with the laws of thermodynamics has been shown before [4, 10, 43]. However, we provide a new approach that offers insight into the connection of a GKSL equation and the individual coefficients of the Hamiltonian H in

Eq. (2.34) by implying thermodynamic considerations to the CM setup instead of applying thermodynamic assumptions to an already existing GKSL equation.
We simply implement the thermodynamic considerations of Section 2.3 by assuming that the interaction defined by the dynamical map in Eq. (2.52) is strictly energy conserving and the environment is initially found in a thermal equilibrium state. Therefore, the unitary interaction between system and environment fulfils SEC as in Eq. (2.72) and the environment is composed out of thermal states τ defined similar to Eq. (2.74) but stationary w.r.t. the environment's free Hamiltonian H_E, such that

$$\tau = \frac{e^{-\beta H_E}}{\mathrm{tr}\left(e^{-\beta H_E}\right)} \tag{2.76}$$

Applying the thermodynamic considerations of this section to the dynamical map in Eq. (2.52) then yields

$$\rho_n = \mathcal{E}\left[\rho_{n-1}\right] = \mathrm{tr}_E\left(U\rho_{n-1}\otimes\tau U^\dagger\right), \tag{2.77}$$

which we will refer to as the thermal map. Here, the environment remains in a thermal state τ (Eq. (2.76)) and the open system Hamiltonian H (Eq. (2.34)), governing the unitary transformation $\mathcal{U}$, fulfils SEC (Eq. (2.72)). The thermal map has the equilibrium property that the thermal state is its fixed point, which can be easily shown by

$$\begin{aligned}
\mathcal{E}\left[\rho_{th}\right] &= \mathrm{tr}_E\left(U\rho_{th}\otimes\tau U^\dagger\right) \\
&= \frac{1}{\mathrm{tr}\left(e^{-\beta H_S}\right)\mathrm{tr}\left(e^{-\beta H_E}\right)}\mathrm{tr}_E\left(e^{-iHt}e^{-\beta(H_S+H_E)}e^{iHt}\right) \\
&= \frac{1}{\mathrm{tr}\left(e^{-\beta H_S}\right)\mathrm{tr}\left(e^{-\beta H_E}\right)}\mathrm{tr}_E\left(e^{-\beta(H_S+H_E)}e^{-iHt}e^{iHt}\right) \\
&= \frac{e^{-\beta H_S}}{\mathrm{tr}\left(e^{-\beta H_S}\right)\mathrm{tr}\left(e^{-\beta H_E}\right)}\mathrm{tr}\left(e^{-\beta H_E}\right) = \rho_{th}.
\end{aligned} \tag{2.78}$$

Here, we used SEC in the second line such that the exponentials commute by them being analytical functions of H and therefore

$$\left[e^{-iHt}, e^{-\beta(H_S+H_E)}\right] = 0. \tag{2.79}$$

By using the dynamical map with these thermodynamic properties to derive the GKSL equation (2.67) following from the Markovian collision model setup

according to Figure 2.6 we find the thermodynamic master equation

$$\boxed{\mathcal{L}[\rho] = -i\left[H_S + H_{LS}, \rho\right] + \Gamma\left(\mathrm{tr}_E\left(V\rho\tau V\right) - \frac{1}{2}\left\{\mathrm{tr}_E(V^2\tau), \rho\right\}\right)}, \quad (2.80)$$

where $H_{LS} = \mathrm{tr}_E\left(H_{SE}\tau\right)$ and $[V, H_S + H_E] = 0$ according to SEC.
We will now study the effects these thermodynamic considerations have on the dynamics of an open quantum system and will see in the end that by letting the map generated by $\mathcal{L}$ act on its fixed point ρ_{th} we will find that the open system's equilibrium conditions can be described by a detailed balance condition.

3 Results

3.1 Steps Towards a Thermodynamic Master Equation

The approach via the collision model allows us to directly relate between the total Hamiltonian in Eq. (2.34) and the Lindblad jump operators appearing in a GKSL master equation in Eq. (2.47). Therefore, the chosen model describes the Markovian system dynamics reliably and we get additional insight into how the individual parts of the total Hamiltonian affect these dynamics.
On the other hand, we have illustrated that to define a dynamical map as in Eq. (2.43), the total Hamiltonian has to satisfy SEC as it is defined in Eq. (2.72). The effects this physically motivated conservation law has on the dynamics of an open quantum system will be worked out in this section. We will do this on hand of the ME resulting from a thermodynamic CM, or thermodynamic master equations as we will refer to them here. Even though these master equations are exactly those that respect strict energy conservation, one does not directly see how the thermodynamic assumptions might affect their structure, at least not when it is in written in the form of Eq. (2.80).
These energy-conserving assumptions allow for a further simplification of the master equation. By that, not only the structure of the equations is changed but also additional insight into its properties is possible. This representation will allow us to directly read off transition rates between energy levels of the system Hamiltonian.
The assumptions taken in this work will allow for even more insight into the dynamics of an open quantum system. It is possible to set the before-found transition rates into a ratio which leads to a detailed balance condition. This ratio can be found by applying the resulting semigroup map (Eq. (2.44)) of a thermodynamic master equation to one of its fixed points, the thermal state. The resulting detailed balance condition then shows that the observed dynamics indeed describe a thermalization process. This behaviour is to be expected since we are dealing with an energy-conserving system.
Following the path and by that also the assumptions taken so far in this work therefore guarantees that strict energy conservation implies detailed balance. The extra insight into the structure of the transition rates appearing in the detailed balance condition will allow us to directly show that detailed balance implies strict energy conservation for some specific but representative cases.
The results in this section can be compared with those of Dann and Kosloff [4]. However, the approach taken in this work is fundamentally different, in that thermodynamic considerations are weaved in right at the beginning of the setup and not directly to a given GKSL equation. Nevertheless, we chose

to use the same notation as in Ref. [4] to allow for direct comparison of the results at intermediate steps. We strive for this section to be self-contained and to keep it that way some calculations can be found in Ref. [4] as well. We decided not to point out every similarity in this section and will discuss the similarities and differences in Section 4.1.1.

3.2 Commutation Relations Following from Strict Energy Conservation

Before it is possible to directly observe the effects of strict energy conservation on the structure of a GKSL equation, we will start by considering the commutation relations of different building blocks of the Lindbladian

$$\mathcal{L}[\rho] = -i \underbrace{[H_S + H_{LS}, \rho]}_{\mathcal{H}[\rho]} + \underbrace{\Gamma \left(\mathrm{tr}_E \left(V\rho \otimes \tau V \right) - \frac{1}{2} \left\{ \mathrm{tr}_E(V^2 \otimes \tau), \rho \right\} \right)}_{\mathcal{D}[\rho]}$$

found in Eq. (2.80) with the system Hamiltonian map $\mathcal{H}_S$. This first step is preliminary to directly observing the effects of strict energy conservation on the structure of the dissipator $\mathcal{D}$. In the later course of this work, these commutation relations will allow us to find an eigenoperator condition for $\mathcal{D}$ by employing the eigenoperator condition of the commuting system unitary map $\mathcal{U}_S$.

3.2.1 Commutation of Dissipator $\mathcal{D}$ and Hamiltonian $\mathcal{H}_S$

We will from now on consider only the dissipative part of the continuous time master equation in Eq. (2.80), which reads

$$\mathcal{D}[\rho] = \Gamma \left(\mathrm{tr}_E \left(V\rho \otimes \tau V \right) - \frac{1}{2} \left\{ \mathrm{tr}_E(V^2 \otimes \tau), \rho \right\} \right). \tag{3.1}$$

It is expressed in terms of the individual Hamiltonians or states that are a function of the Hamiltonians of their respective degrees of freedom. The unscaled interaction Hamiltonian V is part of $H_{SE} = gV$ and the environment thermal state $\tau = e^{-\beta H_E}/Z_E$ is stationary w.r.t its free Hamiltonian H_E. Therefore, this representation will allow for the direct application of the restrictions due to strict energy conservation as stated in Eq. (2.72). In the first step, we will illustrate this behaviour by considering the commutation relations of the maps $\mathcal{H}_S$ and the dissipator $\mathcal{D}$.

The commutation relation between the dissipator $\mathcal{D}$ and the system Hamiltonian map $\mathcal{H}_S$ can be best observed directly by applying these maps on an

arbitrary system state ρ and computing their action by considering $\mathcal{D}[\mathcal{H}_S]$ and $\mathcal{H}_S[\mathcal{D}]$ individually as expressed in

$$\mathcal{D}\left[\mathcal{H}_S\left[\rho\right]\right] = \Gamma\left(\mathrm{tr}_E\left(V\left[H_S,\rho\right]\otimes\tau V\right) - \frac{1}{2}\mathrm{tr}_E\left\{V^2,\left[H_S,\rho\right]\otimes\tau\right\}\right) \tag{3.2}$$

$$\mathcal{H}_S\left[\mathcal{D}\left[\rho\right]\right] = \Gamma\left(\left[H_S,\mathrm{tr}_E\left(V\rho\otimes\tau V\right)\right] - \frac{1}{2}\left[H_S,\mathrm{tr}_E\left\{V^2,\rho\otimes\tau\right\}\right]\right)\ . \tag{3.3}$$

Equivalence between Eqs. (3.2) and (3.3) suffices to show that the maps $\mathcal{D}$ and $\mathcal{H}_S$ commute.
Considering the dissipator in two parts simplifies this proof. We will refer to the first term as the "sandwich" and the second term as the "anti-commutator" term. The sandwich term of Eq. (3.2) can then be rearranged to

$$\begin{aligned}
\mathrm{tr}_E\left(V\left[H_S,\rho\right]\otimes\tau V\right) &= \mathrm{tr}_E\left(VH_S\ \rho\otimes\tau\ V - V\rho\otimes\tau\ H_SV\right)\\
&= \mathrm{tr}_E\big(V(H_S+H_E)\rho\otimes\tau V - V\rho\otimes\tau(H_S+H_E)V\\
&\qquad - VH_E\rho\otimes\tau V + V\rho\otimes\tau H_EV\big)\\
&= \mathrm{tr}_E\left((H_S+H_E)V\rho\otimes\tau V - V\rho\otimes\tau V(H_S+H_E)\right)\\
&= \mathrm{tr}_E\left[H_S,(V\rho\otimes\tau V)\right] + \mathrm{tr}_E\left[H_E,(V\rho\otimes\tau V)\right]\\
&= \left[H_S,\mathrm{tr}_E\left(V\rho\otimes\tau V\right)\right].
\end{aligned} \tag{3.4}$$

In this calculation, we used the fact that H_E and τ commute since the environment thermal state τ is an analytical function of the Hamiltonian H_E. Another property of H_E is that it commutes with $V\rho\otimes\tau V$ within the partial trace over the environment degrees of freedom, even if they do not commute in general. This holds without making any further assumptions on H_E, τ and V. We express the unscaled interaction Hamiltonian V as decomposition in a basis of system and environment by $V=\sum_\alpha A_S^\alpha\otimes B_E^\alpha$ and find that

$$\mathrm{tr}_E\left[H_E,V\rho\otimes\tau V\right] = \sum_{\alpha,\beta} A_S^\alpha\rho A_S^\beta\ \mathrm{tr}\left[H_E,\left(B_E^\alpha\tau B_E^\beta\right)\right] = 0, \tag{3.5}$$

since the commutator is always traceless.
Similarly, we now consider the anti-commutator terms of Eq. (3.2) and see

that they can be transformed into their counterpart in Eq. (3.3) via

$$\begin{aligned}
&\mathrm{tr}_E\left\{V^2,[H_S,\rho]\otimes\tau\right\} = \\
&\quad= \mathrm{tr}_E\left(V^2H_S\rho\otimes\tau - V^2\rho\otimes\tau H_S + H_S\rho\otimes\tau V^2 - \rho\otimes\tau H_S V^2\right) \\
&\quad= \mathrm{tr}_E\big(V^2(H_S+H_E)\rho\otimes\tau - V^2H_E\rho\otimes\tau + \rho\otimes\tau H_E V^2 \\
&\qquad\quad - \rho\otimes\tau(H_S+H_E)V^2 - V^2\rho\otimes\tau H_S + H_S\rho\otimes\tau V^2\big) \\
&\quad= \mathrm{tr}_E\big((H_S+H_E)V^2\rho\otimes\tau - H_EV^2\rho\otimes\tau + \rho\otimes\tau V^2H_E \\
&\qquad\quad - \rho\otimes\tau V^2(H_S+H_E) - V^2\rho\otimes\tau H_S + H_S\rho\otimes\tau V^2\big) \\
&\quad= \mathrm{tr}_E\left(H_SV^2\rho\otimes\tau - \rho\otimes\tau V^2H_S - V^2\rho\otimes\tau H_S + H_S\rho\otimes\tau V^2\right) \\
&\quad= \mathrm{tr}_E\left[H_S,\left\{V^2,\rho\otimes\tau\right\}\right] = \left[H_S,\mathrm{tr}_E\left\{V^2,\rho\otimes\tau\right\}\right].
\end{aligned} \tag{3.6}$$

Similarly, V^2 can be expressed as a sum of tensor products of system and environment parts and it can be shown as in Eq. (3.5) that V^2 commutes with H_E within the partial trace due to the cyclic properties of the trace and commutativity of H_E and τ, i.e.

$$\mathrm{tr}_E\left(V^2H_E\rho\otimes\tau\right) = \mathrm{tr}_E\left(H_EV^2\rho\otimes\tau\right). \tag{3.7}$$

Since both terms of the dissipator commute with the system Hamiltonian as shown in Eqs. (3.4) and (3.6) commutation of the $\mathcal{D}$ and $\mathcal{H}_S$ follows immediately, i.e.

$$\mathcal{D}\left[\mathcal{H}_S\left[\rho\right]\right] = \mathcal{H}_S\left[\mathcal{D}\left[\rho\right]\right]. \tag{3.8}$$

This result also allows for expressing a similar commutation relation of the system unitary map $\mathcal{U}_S = e^{-i\mathcal{H}_S t}$ by employing the fact that if two objects commute, analytical functions of them commute as well. In this case, $\mathcal{U}_S$ is an analytical function of $\mathcal{H}_S$ and the consequences can be summarised as

$$[\mathcal{D},\mathcal{H}_S] = 0 \;\Rightarrow\; [\mathcal{D},\mathcal{U}_S] = 0. \tag{3.9}$$

This commutation relation will prove quite useful in the later course of this work. In section 3.4.1 we will use Eq. (3.9) to find eigenoperator conditions of $\mathcal{D}$ by knowing how $\mathcal{U}_S$ acts on each matrix element $|k\rangle\langle\ell|$ of a system state ρ.

3.2.2 Commutation of Lamb Shift $\mathcal{H}_{LS}$ and Hamiltonian $\mathcal{H}_S$

In this section, we show that commutation of the Lamb shift Hamiltonian $H_{LS} = \mathrm{tr}_E\left(H_{SE}\tau\right)$ as defined in Eq. (2.70) and system Hamiltonian H_S is a direct consequence of strict energy conservation. This result is of particular interest since it is required to show that the Lindbladian map $\mathcal{L} = i(\mathcal{H}_{LS} + \mathcal{H}_S) + \mathcal{D}$ and the system Hamiltonian map $\mathcal{H}_S$ commute. We will also use this

result directly when showing that the thermal state ρ_{th} is a fixed point of the semigroup map Λ_t in Section 3.3.
First, we show that $[H_{LS}, H_S] = 0$ holds. This commutation relation can then be extended to their respective maps $\mathcal{H}_{LS}$ and $\mathcal{H}_S$.
Before showing that $[H_{LS}, H_S] = 0$ directly, we use a as decomposition of $H_{LS} = \sum_\alpha A_\alpha \otimes B_\alpha$ to rearrange the commutator to

$$\begin{aligned}
[H_{LS}, H_S] =& [\mathrm{tr}_E (H_{SE}\tau), H_S] \\
=& \sum_\alpha (A_\alpha H_S \mathrm{tr}(\tau B_\alpha) - H_S A_\alpha \mathrm{tr}(B_\alpha \tau)) \\
=& \mathrm{tr}_E (H_{SE} H_S \otimes \tau - H_S \otimes \tau H_{SE}) \\
=& \mathrm{tr}_E [H_{SE}, H_S \otimes \tau].
\end{aligned} \tag{3.10}$$

To show that the commutator in Eq. (3.10) indeed vanishes we will start with strict energy conservation as given in Eq. (2.72) and apply several transformations to it and see that

$$\begin{aligned}
[H_{SE}, H_S + H_E] = 0 \quad &| \cdot X_E \ |\mathrm{tr}_E \\
\mathrm{tr}_E (H_{SE} H_S X_E + H_{SE} H_E X_E - H_S H_{SE} X_E - H_E H_{SE} X_E) = 0 & \\
\mathrm{tr}_E (H_{SE} H_S X_E + H_{SE} H_E X_E - H_S X_E H_{SE} - H_{SE} H_E X_E) = 0 & \\
\mathrm{tr}_E [H_{SE}, H_S X_E] = 0. &
\end{aligned} \tag{3.11}$$

This calculation is valid for all X_E that commute with the environment Hamiltonian, i.e. they fulfil the commutation relation $[H_E, X_E] = 0$. Therefore, it also holds for $X_E = \tau$. By this choice Eq. (3.11) can be seen to be equivalent to Eq. (3.10) and we can conclude that

$$[H_{LS}, H_S] = 0. \tag{3.12}$$

To see the equivalence between Eq. (3.12) and the commutation relation of the maps, the following calculation suffices

$$\begin{aligned}
\mathcal{H}_{LS}[\mathcal{H}_S[\rho]] &= [H_{LS}, [H_S, \rho]] \\
&= H_{LS} H_S \rho - H_{LS} \rho H_S - H_S \rho H_{LS} + \rho H_S H_{LS} \\
&= H_S H_{LS} \rho - H_S \rho H_{LS} - H_{LS} \rho H_S + \rho H_{LS} H_S \\
&= [H_S, [H_{LS}, \rho]] \\
&= \mathcal{H}_S[\mathcal{H}_{LS}[\rho]].
\end{aligned} \tag{3.13}$$

Hence, by strict energy conservation, the commutation relation of Lamb shift and system Hamiltonian map $\mathcal{H}_{LS}[\mathcal{H}_S[\rho]] = \mathcal{H}_S[\mathcal{H}_{LS}[\rho]]$ holds.

3.2.3 Commutation of the Unitary $\mathcal{U}_S$ and the Semigroup Map Λ_t

To better compare our results to those of Ref. [4], we show that the maps Λ_t and $\mathcal{U}_S$ commute.
By using the commutation relations in Eqs. (3.8) and (3.13) we can now conclude that the Lindbladian $\mathcal{L} = -i(\mathcal{H}_{LS}+\mathcal{H}_S)+\mathcal{D}$ commutes with the system Hamiltonian map $\mathcal{H}_S$, i.e.

$$[\mathcal{L}, \mathcal{H}_S] = [-i\left(\mathcal{H}_S + \mathcal{H}_{LS}\right) + \mathcal{D}, \mathcal{H}_S] = -i\left[\mathcal{H}_{LS}, \mathcal{H}_S\right] + [\mathcal{D}, \mathcal{H}_S] = 0. \quad (3.14)$$

The commutation relation of the maps $\Lambda_t = e^{\mathcal{L}t}$ and $\mathcal{U}_S = e^{-i\mathcal{H}_S t}$ follows from the commutation relation of their generators $\mathcal{L}$ and $\mathcal{H}_S$ in Eq. (3.14). Employing that the maps of interest are analytical functions of their generators yields

$$[\mathcal{L}, \mathcal{H}_S] = 0 \;\Rightarrow\; [\Lambda_t, \mathcal{U}_S] = \left[e^{\mathcal{L}t}, e^{-i\mathcal{H}_S t}\right] = 0. \quad (3.15)$$

We want to emphasise again that this is a direct consequence of strict energy conservation.
All results that are needed for the following calculations were already found in Eqs. (3.9) and (3.12). It is still not obvious how these commutation relations will help to gain more insight into the open system dynamics following a GKSL master equation. However, the fundamental consequences of strict energy conservation that are already embedded in Eq. (3.9) will reveal themselves in the calculations of Section 3.4.

3.3 Fixed Point of the Semigroup Map Λ_t

In Section 2.1.2 we introduced the dynamical map $\mathcal{E}$ in Eq. (2.77), which doesn't necessarily lead to the same dynamics as the semigroup map in Eq. (2.44) as we showcased in an example in Appendix B.1. However, in Eq. (2.78) we find the fixed point of the thermal map, the thermal state ρ_{th} at the same inverse temperature β as the environment. We will now show that this also holds for the semigroup map Λ_t generated by the Lindbladian $\mathcal{L}$ in Eq. (2.80). To show the fixed point condition $\Lambda_t[\rho_{th}] = \rho_{th}$ we will let the individual terms of $\mathcal{L}$ act on the system thermal state ρ_{th} and see afterwards that vanishing action of $\mathcal{L}$ on ρ_{th} indeed leads to a fixed point of the map Λ_t.
We start by considering the product of the un-normalized thermal states of system and environment at equilibrium. This expression can be simplified to

$$e^{-\beta H_S} e^{-\beta H_E} = e^{-\beta(H_S+H_E)}, \quad (3.16)$$

since the Hamiltonians H_S and H_E act on different subspaces and by that they trivially commute.
Computing the commutator of the interaction Hamiltonian H_{SE} and the product in Eq. (3.16) can then be simplified to

$$\left[H_{SE}, e^{-\beta H_S} e^{-\beta H_E}\right] = \left[H_{SE}, e^{-\beta(H_S+H_E)}\right] = 0 \;\Rightarrow\; [V, \rho_{th} \otimes \tau] = 0, \quad (3.17)$$

by employing SEC. Before we show that the action of $\mathcal{L}$ on ρ_{th} vanishes, we first let $\mathcal{D}$ act on ρ_{th} and see that

$$\begin{aligned} \mathcal{D}[\rho_{th}] &= \Gamma\left(\mathrm{tr}_E\left(V\rho_{th}\otimes\tau V\right) - \frac{1}{2}\mathrm{tr}_E\left\{V^2, \rho_{th}\otimes\tau\right\}\right) \\ &= \Gamma\left(\mathrm{tr}_E\left(V^2\rho_{th}\otimes\tau\right) - \frac{1}{2}\mathrm{tr}_E\left(2V^2\rho_{th}\otimes\tau\right)\right) = 0, \end{aligned} \quad (3.18)$$

due to the result of Eq. (3.17). In Eq. (3.12) we have already shown that the Lamb shift Hamiltonian map $\mathcal{H}_{LS}$ and the system Hamiltonian map $\mathcal{H}_S$ commute. By that, the action of the Lindbladian $\mathcal{L}$ on the thermal state vanishes, and the following calculation suffices to show that

$$\mathcal{L}[\rho_{th}] = -i\left(\mathcal{H}_S[\rho_{th}] + \mathcal{H}_{LS}[\rho_{th}]\right) + \mathcal{D}[\rho_{th}] = 0. \quad (3.19)$$

Here we used $\mathcal{H}_{LS}[\rho_{th}] = \frac{1}{Z_S}\left[H_{LS}, e^{-\beta H_S}\right] = 0$ by virtue of Eq. (3.12). The same reasoning suffices to show that $\mathcal{H}_S[\rho_{th}] = 0$, since the system thermal state ρ_{th} is stationary w.r.t. its free Hamiltonian H_S.
To see that the thermal state is a fixed point of the semigroup map Λ_t we will express the action of the map in a series expansion. With help of Eq. (3.19) we see that

$$e^{\mathcal{L}t}[\rho_{th}] = \sum_i \frac{(\mathcal{L}t)^i}{i!}[\rho_{th}] = \left(\mathcal{I}[\rho_{th}] + \mathcal{L}[\rho_{th}]\, t + \frac{\mathcal{L}[\mathcal{L}[\rho_{th}]]\, t^2}{2} + \cdots\right) = \rho_{th}. \quad (3.20)$$

The result shows that any state for which the action of the Lindbladian $\mathcal{L}$ vanishes is a fixed point of the semigroup map Λ_t and therefore also holds for the thermal state ρ_{th}, i.e.

$$\boxed{\Lambda_t[\rho_{th}] = \rho_{th}}. \quad (3.21)$$

We will later employ the fixed point of the semigroup map Λ_t to find a detailed balance condition for the coefficients appearing in the master equation, similar to the DB condition in Eq. (2.75) we found for a classical master equation.

3.4 Study of the Action of $\mathcal{D}$ on Basis Elements of $\mathcal{U}_S$

In Section 3.2.1 we found the commutation relation for the dissipator $\mathcal{D}$ of a thermodynamic master equation and the system unitary map $\mathcal{U}_S$,

$$[\mathcal{D}, \mathcal{U}_S] = 0.$$

Since the maps $\mathcal{U}_S$ and $\mathcal{D}$ commute, they share a common set of eigenoperators. But we will soon see that the spectrum of $\mathcal{U}_S$ is degenerate, which requires a more detailed consideration of how $\mathcal{D}$ acts on the eigenoperators of $\mathcal{U}_S$. More precisely, the diagonal elements of $\mathcal{U}_S$'s spectrum constitute the degenerate part and the off-diagonal elements the non-degenerate part. In the end, this distinction allows for eliminating terms the GKSL equation and expressing it in its thermodynamic essential form.

3.4.1 Analysing the Action of the Maps on Distinct Basis Elements

To motivate this classification, we will first consider the action of $\mathcal{U}_S$ on a general basis element $|n\rangle\langle m|$ where $|n\rangle, |m\rangle$ are eigenvectors of H_S. According to Eq. (2.25) this unitary evolution is given by

$$\begin{aligned}
\mathcal{U}_S\left[|n\rangle\langle m|\right] =& e^{-iH_S t}|n\rangle\langle m| e^{iH_S t} \\
=& \sum_{k,j} e^{-i\varepsilon_k t}|k\rangle\langle k|n\rangle\langle m| e^{i\varepsilon_j t}|j\rangle\langle j| \\
=& e^{i(\varepsilon_m-\varepsilon_n)t}|n\rangle\langle m| \\
=& e^{i\omega_{nm}t}|n\rangle\langle m|.
\end{aligned} \tag{3.22}$$

Here we used the definition of the Bohr frequency ω_{nm} between the energy levels $|n\rangle$ and $|m\rangle$, as given in Eq. (2.16). It can now be seen that Eq. (3.22) constitutes an eigenoperator condition with eigenvalue $e^{i\omega_{nm}t}$ for all n, m. The degeneracies of the eigenoperators of $\mathcal{U}_S$ can be best observed when separating them into two distinct sets. These will be named based on how the map $\mathcal{U}_S$ acts on them. First, there is the set that contains projection operators $\Pi_i = |i\rangle\langle i|$. This set is referred to as *unitarily invariant* since

$$\mathcal{U}_S\left[\Pi_i\right] = \Pi_i \quad \forall i \tag{3.23}$$

constitutes a d_S-fold degenerate eigenoperator condition with eigenvalue 1. The set containing transition operators $F_{nm} = |n\rangle\langle m|$ for $n \neq m$ is referred to as *unitarily non-invariant* and fulfils the following eigenoperator condition

$$\mathcal{U}_S\left[F_{nm}\right] = e^{i\omega_{nm}t}F_{nm}. \tag{3.24}$$

For these eigenoperators, we assume nondegeneracy of their corresponding eigenvalues $e^{i\omega_{nm}t}$. This means that the Bohr frequencies as in Eq. (2.16) between energy level $|n\rangle$ and $|m\rangle$ of the system Hamiltonian H_S are non-degenerate, i.e. $\omega_{nm} \neq \omega_{n'm'}$ for all $(n,m) \neq (n',m')$. One direct consequence thereof is that the spectrum of H_S composed of eigenvalues ε_i is also non-degenerate. However, even non-degenerate H_S can still lead to degenerate Bohr frequencies if e.g. two different pairs of eigenvalues exhibit the same energy gap.

Classifying the entire spectrum of H_S into a degenerate and a non-degenerate part w.r.t the eigenoperator condition of $\mathcal{U}_S$ in Eq. (3.22) will allow us to make statements on how the dissipator $\mathcal{D}$ acts on these parts individually by also employing the commutation relation of $\mathcal{U}_S$ and $\mathcal{D}$ found in Eq. (3.9).

If two observables commute then there exists a common eigenbasis. If these operators are additionally non-degenerate then this eigenbasis is unique. A similar statement can be made about commuting maps. The action of $\mathcal{D}$ on the unitary non-invariant (non-degenerate) part of the spectrum yields a unique eigenoperator condition on the same basis as for $\mathcal{U}_S$. Therefore, Eqs. (3.9) and (3.24) imply

$$\mathcal{D}\left[F_{nm}\right] = f_{nm}F_{nm} \qquad \forall\ n \neq m. \tag{3.25}$$

If at least one of two commuting observables is degenerate to some degree, then the eigenspace of the other observable is typically spanned by a linear combination of the basis elements of the degenerate one. Applied to the maps at hand, this is the case for the degenerate unitary invariant part of the spectrum of $\mathcal{U}_S$. This means that Eqs. (3.9) and (3.23) imply that

$$\mathcal{D}\left[\Pi_n\right] = \sum_i d_i^{(n)} \Pi_i. \tag{3.26}$$

The coefficients $d_i^{(n)}$ and f_{nm} could be computed explicitly once H_S, H_E and H_{SE} are known, but since their actual value is of no significance we will leave them unspecified.

Knowing how $\mathcal{D}$ acts on the elements of the eigenbasis of H_S is necessary for an analysis of coefficient contributions to the open system dynamics, which will be performed in Section 3.5.3. In this analysis, we will find out if some of the coefficients f_{nm} and $d_i^{(n)}$ vanish and by that restrict the structure of the resulting thermodynamic master equation.

3.5 Thermodynamic GKSL Equation

3.5.1 Basis Change of the Dissipator

In this section, we will determine which terms in the dissipator contribute to the overall dynamics and can reduce the dissipator to its thermodynamically essential form, which leads to the thermodynamic master equation.
Considering the dissipator in its dual form helps to compare our calculations to those in Ref. [4], but also slightly simplifies the notation. The dual form can be found by employing the Hilbert Schmidt product of an arbitrary Hermitian operator A and the map in its primal form acting on a state ρ. This can then be transformed to

$$\begin{aligned}
\operatorname{tr}\left(\mathcal{D}\left[\rho\right]A\right) &= \operatorname{tr}\left(\sum_{\mu,\nu}\left(L_{\mu\nu}\rho L_{\mu\nu}^{\dagger} - \frac{1}{2}\left\{L_{\mu\nu}^{\dagger}L_{\mu\nu},\rho\right\}\right)A\right) \\
&= \operatorname{tr}\left(\sum_{\mu,\nu}\left(L_{\mu\nu}^{\dagger}AL_{\mu\nu}\rho - \frac{1}{2}\left(L_{\mu\nu}^{\dagger}L_{\mu\nu}A\rho + AL_{\mu\nu}^{\dagger}L_{\mu\nu}\rho\right)\right)\right) \\
&= \operatorname{tr}\Bigg(\underbrace{\sum_{\mu,\nu}\left(L_{\mu\nu}^{\dagger}AL_{\mu\nu} - \frac{1}{2}\left\{L_{\mu\nu}^{\dagger}L_{\mu\nu},A\right\}\right)}_{=:\mathcal{D}^{*}\left[A\right]}\rho\Bigg) = \operatorname{tr}\left(\mathcal{D}^{*}\left[A\right]\rho\right).
\end{aligned} \tag{3.27}$$

Here, we used the fact that A and ρ are Hermitian operators, that the dissipator is Hermitianity preserving ($\mathcal{D}\left[A\right] = \left(\mathcal{D}\left[A\right]\right)^{\dagger}$) and employed the cyclic properties of the trace. Therefore, the dissipator in its dual form $\mathcal{D}^{*}$ reads

$$\mathcal{D}^{*}\left[\bullet\right] = \sum_{\mu,\nu}\left(L_{\mu\nu}^{\dagger}\bullet L_{\mu\nu} - \frac{1}{2}\left\{L_{\mu\nu}^{\dagger}L_{\mu\nu},\bullet\right\}\right). \tag{3.28}$$

To eliminate elements of the dissipator that don't contribute to the dynamic evolution of the system, we will next perform an analysis of coefficient contributions to these dynamics. Expressing Eq. (3.28) in a basis of orthogonal matrices S_i will be used to define coefficients for each index combination. Orthonormality can be defined by the Hilbert-Schmidt product $\left(S_i, S_j\right) = \operatorname{tr}\left(S_i^{\dagger}S_j\right) = \delta_{ij}$. The Lindblad jump operators on the basis of these orthonormal matrices are then given by

$$L_{\mu\nu} = \sum_{i=0}^{d_S^2-1}\left(L_{\mu\nu},S_i\right)S_i. \tag{3.29}$$

Plugging Eq. (3.29) into Eq. (3.28) gives the dissipator in the basis of these orthonormal operators

$$\mathcal{D}^*\left[\bullet\right] = \sum_{j,i}\sum_{\mu,\nu}\left(L_{\mu\nu}, S_j\right)^*\left(L_{\mu\nu}, S_i\right)\left(S_j^\dagger \bullet S_i - \frac{1}{2}\left\{S_j^\dagger S_i, \bullet\right\}\right). \tag{3.30}$$

By collecting scalar terms in Eq. (3.30) we define the coefficients

$$a_{ji} := \sum_{\mu,\nu}\left(L_{\mu\nu}, S_j\right)^*\left(L_{\mu\nu}, S_i\right). \tag{3.31}$$

With the help of these, we express the dissipator in a compact form as

$$\mathcal{D}^*\left[\bullet\right] = \sum_{j,i} a_{ji}\left(S_j^\dagger \bullet S_i - \frac{1}{2}\left\{S_j^\dagger S_i, \bullet\right\}\right). \tag{3.32}$$

We choose $S_j = |m\rangle\langle n|$ and $S_i = |n'\rangle\langle m'|$ and plug them into Eq. (3.31). These operators are orthonormal according to the Hilbert-Schmidt product and cover diagonal elements Π_i as well as off-diagonal elements F_{nm}. Therefore, the set of orthogonal matrices $\{S\}$ spans over the entire eigenspace of $\mathcal{U}_S$, where $\{|m\rangle\langle n|\}$ forms a complete basis that is also orthonormal.
The action of the dissipator can then be expressed in terms of the new indices $j \to (n, m)$ and $i \to (n', m')$. The sum over these indices shows $\mathcal{D}^*$ in the abstract form

$$\mathcal{D}^*\left[\bullet\right] = \sum_{n,m,n',m'} a_{nmn'm'}\mathcal{D}^*_{nmn'm'}\left[\bullet\right]. \tag{3.33}$$

The partial dissipator maps $\mathcal{D}^*_{nmn'm'}$ appearing in Eq. (3.33) can be obtained by plugging the operators $S_j = |n\rangle\langle m|$ and $S_i = |n'\rangle\langle m'|$ into the unscaled part of Eq. (3.32) and read

$$\mathcal{D}^*_{nmn'm'}\left[\bullet\right] = |n\rangle\langle m| \bullet \left|n'\right\rangle\left\langle m'\right| - \frac{1}{2}\left\{|n\rangle\langle m|n'\rangle\left\langle m'\right|, \bullet\right\}. \tag{3.34}$$

We introduce these partial maps together with the four index coefficients $a_{nmn'm'}$ to determine the action on individual basis elements for different index combinations (n, m, n', m'). Considering these elements individually will enable us to tell which of these partial maps contribute to the overall dynamics and which do not. In the end this results in a thermodynamically essential form of the master equation.
The coefficients $a_{nmn'm'}$ appearing in Eq. (3.33) replace the two index coefficients a_{ji}. To see this we again plug the explicit orthonormal operators $S_j = |m\rangle\langle n|$ and $S_i = |n'\rangle\langle m'|$ into Eq. (3.31) and find

$$a_{nmn'm'} = \sum_{\mu,\nu}\left(L_{\mu\nu}, |m\rangle\langle n|\right)^*\left(L_{\mu\nu}, \left|n'\right\rangle\left\langle m'\right|\right). \tag{3.35}$$

The $L_{\mu\nu}$ are the Lindblad jump operators that follow from the collision model and were introduced in Eq. (2.61). They allow us to relate the four-index coefficients $a_{nmn'm'}$ to the elements of the Hamiltonians in Eq. (2.34). To illustrate this step, one individual Hilbert-Schmidt product of Eq. (3.35) can be evaluated to

$$\begin{aligned}(L_{\mu\nu}, |m\rangle\langle n|) &= \mathrm{tr}\left(L_{\mu\nu}^{\dagger}|m\rangle\langle n|\right) \\ &= \sqrt{p_\nu}\mathrm{tr}\left(\langle\nu|V|\mu\rangle|m\rangle\langle n|\right) \\ &= \sqrt{p_\nu}\sum_{i,j,\xi,\chi}\mathrm{tr}\left(\langle\nu|c_{i\xi j\chi}|i\rangle\langle j|\otimes|\xi\rangle\langle\chi|\,|\mu\rangle|m\rangle\langle n|\right) \\ &= \sqrt{p_\nu}\sum_{i}c_{i\nu m\mu}\underbrace{\mathrm{tr}\left(|i\rangle\langle n|\right)}_{=\delta_{in}} \\ &= \sqrt{p_\nu}c_{n\nu m\mu}.\end{aligned} \tag{3.36}$$

Here, the coefficients p_ν are the eigenvalues of the environment thermal state τ and $c_{n\nu m\mu}$ are the elements of the unscaled interaction Hamiltonian V. This result can be plugged into the Hilbert Schmidt products in the definition of the four index coefficients $a_{nmn'm'}$ as stated in Eq. (3.35). The $a_{nmn'm'}$ can then be evaluated in terms of the coefficients p_ν and $c_{i\mu j\nu}$ to

$$a_{nmn'm'} = \sum_{\mu\nu}(L_{\mu\nu}, |m\rangle\langle n|)^*\left(L_{\mu\nu}, |n'\rangle\langle m'|\right) = \sum_{\mu,\nu}p_\nu c^*_{n\nu m\mu}c_{m'\nu n'\mu}. \tag{3.37}$$

Letting the maps in Eq. (3.34) act on an operator $|k\rangle\langle\ell|$ will give an idea of what the action of the map on a state ρ looks like. The action of the partial dissipator map on individual basis elements can be expressed as

$$\begin{aligned}&\mathcal{D}^*_{nmn'm'}[|k\rangle\langle\ell|] = \\ &\quad= |n\rangle\langle m|k\rangle\langle\ell|n'\rangle\langle m'| - \frac{1}{2}\langle m|n'\rangle\left(|n\rangle\langle m'|k\rangle\langle\ell| + |k\rangle\langle\ell|n\rangle\langle m'|\right) \\ &\quad= \delta_{km}\delta_{\ell n'}|n\rangle\langle m'| - \frac{1}{2}\delta_{mn'}\left(\delta_{km'}|n\rangle\langle\ell| + \delta_{\ell n}|k\rangle\langle m'|\right).\end{aligned} \tag{3.38}$$

Considering how $\mathcal{D}^*_{nmn'm'}$ maps onto an individual matrix element $|k'\rangle\langle\ell'|$ reveals

$$\begin{aligned}&\langle k'|\,\mathcal{D}_{nmn'm'}\left[|k\rangle\langle\ell|\right]|\ell'\rangle = \\ &\qquad= \delta_{nk'}\delta_{km}\delta_{\ell n'}\delta_{m'\ell'} - \frac{1}{2}\delta_{mn'}\left(\delta_{k'n}\delta_{km'}\delta_{\ell\ell'} + \delta_{\ell n}\delta_{m'\ell'}\delta_{k'k}\right)\end{aligned} \tag{3.39}$$

The work done in this section is preliminary to performing an analysis of

coefficient contributions to the open system dynamics, where the action of the map $\mathcal{D}^*$ on elements from the invariant and non-invariant spectrum of $\mathcal{U}_S$ will be evaluated. To tell which index combinations contribute to the overall dynamics and which do not, Eq. (3.39) will prove itself useful. The elements that do not contribute to the dynamics can then subsequently be removed from the sum in Eq. (3.33) and the dissipator in its thermodynamically essential form is constructed of the remaining coefficients $a_{nmn'm'}$ and partial maps $\mathcal{D}^*_{nmn'm'}$. It will be possible to separate the remaining coefficients into two distinct sets that each show properties that allow for more insight into the dynamics of the open quantum system.

3.5.2 Consequences of Strict Energy Conservation on Elements of the Dissipator

The calculation of this section aims to make out for which combinations of indices, the coefficients $a_{nmn'm'}$ vanish due to strict energy conservation. Therefore, we will highlight exactly how strict energy conservation affects the structure of the dissipator. This will be done in line with the restrictions that follow from the commutation of $\mathcal{U}_S$ and $\mathcal{D}$ given in Eqs. (3.25) and (3.26). These effects will be considered separately for elements of the invariant and non-invariant spectrum, which will then be combined to see a complete picture in the end.

First, we observe the action of the dissipator on elements of the unitary non-invariant spectrum, i.e. transition operators F_{nm}. While Eq. (3.38) already reveals how the dissipator acts on a general basis element. We will take one step back and start by bringing Eqs. (3.25) and (3.33) together to obtain

$$\left\langle k' \right| \sum_{n,m,n',m'} a_{nmn'm'} \mathcal{D}_{nmn'm'} \left[\left| k \right\rangle \left\langle \ell \right| \right] \left| \ell' \right\rangle \stackrel{!}{=} \left\langle k' \right| f_{kl} \left| k \right\rangle \left\langle \ell \right| \left| \ell' \right\rangle \qquad \forall\ k \neq \ell. \tag{3.40}$$

Plugging the results of Eq. (3.39) into Eq. (3.40) summarises the relation between the four-index coefficients $a_{nmn'm'}$ and the eigenvalues $f_{k\ell}$ in the following way

$$a_{k'k\ell\ell'} - \frac{1}{2} \sum_m \left(a_{k'mmk} \delta_{\ell\ell'} + a_{\ell mm\ell'} \delta_{kk'} \right) = f_{k\ell} \delta_{kk'} \delta_{\ell\ell'} \qquad \forall k \neq \ell. \tag{3.41}$$

Next, we will consider the action of the dissipator on elements of the invariant spectrum, i.e. diagonal elements Π_i. To achieve this, we first need to set

Eqs. (3.26) and (3.33) equivalent, resulting in

$$\langle k' | \sum_{n,m,n',m'} a_{nmn'm'} \mathcal{D}_{nmn'm'} \left[|k\rangle \langle k| \right] |\ell'\rangle \stackrel{!}{=} \langle k' | \left(\sum_i b_i^{(k)} |i\rangle \langle i| \right) |\ell'\rangle . \quad (3.42)$$

Similarly as before, by plugging Eq. (3.39) into Eq. (3.42), but this time setting $k = \ell$, we find another condition between proportionality constants $b_i^{(n)}$ of Eq. (3.26) and four index coefficients $a_{nmn'm'}$ of Eq. (3.33) of the following form

$$a_{k'kk\ell'} - \frac{1}{2} \sum_m \left(a_{k'mmk} \delta_{k\ell'} + a_{kmm\ell'} \delta_{kk'} \right) = b_{k'}^{(k)} \delta_{\ell' k'}. \quad (3.43)$$

The Kronecker deltas δ_{ij} in Eqs. (3.41) and (3.43) govern which pairs of indices of the coefficients $a_{ijk\ell}$ are set to be equivalent. It is hard to make any statements about these coefficients by directly looking at Eqs. (3.41) and (3.43). Up until now, it is not clear how these conditions, which are again a consequence of strict energy conservation, will alter the structure of a GKSL master equation. To gain more insight into their implications, we will perform a thorough analysis of coefficient contributions to the open system dynamics in the next section. The final result of this analysis will show which terms of the master equation contribute to the open system dynamics and which vanish due to the thermodynamic setup of the CM.

3.5.3 Analysis of Coefficient Contributions to the Open System Dynamics

In this case study we considered all possible index combinations in Eqs. (3.41) and (3.43). The calculations that lead to the results can be found in Appendix E.1. Here, we present the results in a concise form in Tables 1 and 2. To make this more accessible, we repeat the relevant equations from Appendix E.1 above each table.

$$a_{k'kk\ell'} - \frac{1}{2} \sum_m \left(a_{k'mmk} \delta_{k\ell'} + a_{kmm\ell'} \delta_{kk'} \right) = b_{k'}^{(k)} \delta_{\ell' k'}.$$

$$a_{k'k\ell\ell'} - \frac{1}{2} \sum_m \left(a_{k'mmk} \delta_{\ell\ell'} + a_{\ell mm\ell'} \delta_{kk'} \right) = f_{k\ell} \delta_{kk'} \delta_{\ell\ell'} \ \forall k \neq \ell.$$

To give meaning to Tables 1 and 2, we want to emphasize that they summarize the results of an evaluation of all the coefficients $a_{nmn'm'}$ that can be non-zero while still satisfying the eigenoperator Eqs. (3.41) and (3.43).

Cases			Contributing Elements	Reference
$k = \ell$				(3.43)
	$k' \neq \ell'$			(E.1)
		$k \neq k'$ and $k \neq \ell'$	none	(E.2)
		$k = \ell' \Rightarrow k \neq k'$	$a_{k\ell\ell\ell}, a_{kkk\ell}\ \forall k \neq \ell$	(E.3)
		$k = k' \Rightarrow k \neq \ell'$	$a_{k\ell\ell\ell}, a_{kkk\ell}\ \forall k \neq \ell$	(E.4)
	$k' = \ell'$			(E.5)
		$k = k'$	$a_{k\ell\ell k}\ \forall k \neq \ell$	(E.6)
		$k \neq k'$	$a_{k\ell\ell k}\ \forall k \neq \ell$	(E.7)

Table 1: Results of the case study considering the action of $\mathcal{D}$ on the invariant part of the spectrum

Cases		Contributing Elements	Reference
$k \neq \ell$			(3.41)
	$k = k'$ and $\ell \neq \ell'$	$a_{kk\ell m}, a_{k\ell\ell\ell}, a_{kkk\ell}\ \forall k \neq \ell, \ell \neq m$	(E.10)
	$k \neq k'$ and $\ell = \ell'$	$a_{k\ell mm}, a_{k\ell\ell\ell}, a_{kkk\ell}\ \forall k \neq \ell, \ell \neq m$	(E.11)
	$k \neq k'$ and $\ell \neq \ell'$	none	(E.12)
	$k = k'$ and $\ell = \ell'$	$a_{kk\ell\ell}, a_{kmmk}\ \forall k \neq \ell$	(E.13)

Table 2: Results of the case study considering the action of $\mathcal{D}$ on the non-invariant part of the spectrum

This case study reveals which terms of the dissipator vanish due to eigenoperator commutation relations following from strict energy conservation. It additionally shows how the remaining terms are related to each other. We also copied the final result of the case study in Eq. (E.18) to present it here

$$a_{kkk\ell} = a_{k\ell\ell\ell} = a_{k\ell nn} = a_{mmk\ell}\ \forall\ k \neq \ell,\ \ell \neq n,\ k \neq m. \tag{3.44}$$

This tells us that all the surviving coefficients except $a_{kk\ell\ell}$ and $a_{k\ell\ell k}$ need to coincide but not necessarily vanish to fulfil the initial conditions on how the dissipator $\mathcal{D}$ acts on the elements of a basis according to Eqs. (3.25) and (3.26). Hence, up until this point it is not clear if the coefficients in Eq. (3.44) contribute to the dynamics since they coincide but don't necessarily vanish. Therefore, they need to be considered in the structure of the dissipator for now. However, we will soon see that the requirement for them to coincide also sharply restricts their contribution to the overall system dynamics.
To summarise, all the terms that can be found in a dissipator that still complies with strict energy conservation read

- $a_{kk\ell\ell}$ for $k \neq \ell$ and $a_{k\ell\ell k}$ for all k, ℓ from Eqs. (E.4), (E.7) and (E.13) .
- $a_{kkk\ell},\ a_{k\ell\ell\ell},\ a_{k\ell nn},\ a_{mmk\ell}\ \forall\ k \neq \ell,\ \ell \neq n,\ k \neq m$ combined in Eq. (3.44)

Here the separation into these two distinct sets is chosen intentionally and the calculation in the next section will justify this choice.

3.5.4 Contributions to the Overall Dynamics

We will now see that all the terms in the dissipator except $a_{k\ell\ell k}$ and $a_{kk\ell\ell}$ are insignificant since they do not contribute to the overall dynamics. By considering the dissipator composed of the non-vanishing coefficients found in Section 3.5.3 we will find which elements contribute by plugging in Eq. (3.34) into Eq. (3.33) to find that

$$\begin{aligned}
\mathcal{D}^*[\bullet] = &\sum_{k,\ell} a_{kk\ell\ell}\left(|k\rangle\langle k|\bullet|\ell\rangle\langle\ell| - \frac{1}{2}\{|k\rangle\langle k|\ell\rangle\langle\ell|, \bullet\}\right) \\
&+ \sum_{k\neq\ell} a_{k\ell\ell k}\left(|k\rangle\langle\ell|\bullet|\ell\rangle\langle k| - \frac{1}{2}\{|k\rangle\langle\ell|\ell\rangle\langle k|, \bullet\}\right) \\
&+ \sum_{k\neq\ell} a_{kkk\ell}\left(|k\rangle\langle k|\bullet|k\rangle\langle\ell| - \frac{1}{2}\{|k\rangle\langle k|k\rangle\langle\ell|, \bullet\}\right) \\
&+ \sum_{k\neq\ell} a_{k\ell\ell\ell}\left(|k\rangle\langle\ell|\bullet|\ell\rangle\langle\ell| - \frac{1}{2}\{|k\rangle\langle\ell|\ell\rangle\langle\ell|, \bullet\}\right) \\
&+ \sum_{k\neq\ell,\ell\neq m} a_{k\ell mm}\left(|k\rangle\langle\ell|\bullet|m\rangle\langle m| - \frac{1}{2}\{|k\rangle\langle\ell|m\rangle\langle m|, \bullet\}\right) \\
&+ \sum_{k\neq\ell,\ell\neq m} a_{kk\ell m}\left(|k\rangle\langle k|\bullet|\ell\rangle\langle m| - \frac{1}{2}\{|k\rangle\langle k|\ell\rangle\langle m|, \bullet\}\right)
\end{aligned} \tag{3.45}$$

We want to note here that we moved the index combination $k = \ell$ from the second line ($a_{k\ell\ell k}$), to the sum in the first line ($a_{kk\ell\ell}$) by exchanging the summation indices $k \neq \ell$ and k, ℓ in these two lines. This shift of the indices will prove itself convenient later when the remaining operators in the dissipator are grouped based on the way they act on input states.

To see which terms contribute to the overall dynamics and for which the action vanishes, it is convenient to let Eq. (3.45) act on basis elements of the invariant and non-invariant spectrum of $\mathcal{U}_S$ separately. To isolate the individual contributions of the found index combinations to the dynamics, we will treat each line of Eq. (3.45) individually. The full calculation can be found in Appendix E.2. Nevertheless, we choose to present the third line of Eq. (3.45) on an element $|i\rangle\langle j|$ for $i \neq j$ as a show-case example

$$\begin{aligned}\sum_{k\neq\ell} a_{kkk\ell}\left(|k\rangle\langle k|i\rangle\langle j|k\rangle\langle\ell| - \frac{1}{2}\left\{|k\rangle\langle k|k\rangle\langle\ell|, |i\rangle\langle j|\right\}\right)\\ = -\frac{1}{2}\left(\sum_k a_{kkki}|k\rangle\langle j| + \sum_\ell a_{jjj\ell}|i\rangle\langle\ell|\right),\end{aligned} \tag{3.46}$$

where we evaluated the inner products and applied the resulting Kronecker deltas to the coefficients. Similar calculations for the other lines can be found in Eqs. (E.19) to (E.22). By applying the restriction in Eq. (3.44) on the four index coefficients $a_{nmn'm'}$ we indeed find that the lines in Eq. (3.45) with coefficients $a_{kkk\ell}, a_{k\ell\ell\ell}, a_{k\ell mm}$ and $a_{kk\ell m}$ cancel each other. The calculation can be found in Eq. (E.23) in Appendix E.2. Similar calculations for Eq. (3.45) acting on projection operators Π_i can be found in Eqs. (E.24) to (E.27). The lines in Eq. (3.45) with coefficients $a_{kkk\ell}, a_{k\ell\ell\ell}, a_{k\ell mm}$ and $a_{kk\ell m}$ also vanish by employing Eq. (3.44), which can be seen in Eq. (E.28)
By that, we see that all lines except the first and second one of Eq. (3.45) vanish when considering their joint action on any given basis element. Since this covers the action of the map on an entire operator basis, these two lines represent the overall dynamics governed by the dissipator. We will then be able to state the thermodynamic essential form of the dissipator only consisting of the lines with coefficients of the form $a_{k\ell\ell k}$ and $a_{kk\ell\ell}$ in Eq. (3.47). This result of strict energy conservation will allow for directly observing the effects it has on the structure of the master equation.

3.5.5 Thermodynamic Essential Structure of the Dissipator $\mathcal{D}$

Up until now, we found that out of the index combinations $a_{nmn'm'}$ only the ones of the form $a_{kk\ell\ell}$ and $a_{k\ell\ell k}$ contribute to the overall dynamics. In every step that led up to this point, the actual values of these coefficients were of no significance and we only found out which terms contribute and which do not. Due to Eq. (3.37) we know how they are related to H_S, H_E and H_{SE} and we will now illustrate their physical significance.
The non-vanishing lines of Eq. (3.45) describe the overall dynamics and lead to the thermodynamic essential dissipator of the form

$$\begin{aligned}\mathcal{D}^*[\bullet] = &\sum_{k,\ell} a_{kk\ell\ell}\left(|k\rangle\langle k|\bullet|\ell\rangle\langle\ell| - \frac{1}{2}\left\{|k\rangle\langle k|\ell\rangle\langle\ell|, \bullet\right\}\right)\\ &+\sum_{k\neq\ell} a_{k\ell\ell k}\left(|k\rangle\langle\ell|\bullet|\ell\rangle\langle k| - \frac{1}{2}\left\{|k\rangle\langle\ell|\ell\rangle\langle k|, \bullet\right\}\right)\end{aligned} \tag{3.47}$$

To simplify this equation we will express it in terms of transition operators

$F_{k\ell} = |k\rangle\langle\ell|$ for $k \neq \ell$ and projection operators $\Pi_k = |k\rangle\langle k|$. We will also define the two different combinations of four index coefficients as $a_{kk\ell\ell} \equiv \alpha_{k\ell}$ and $a_{k\ell\ell k} \equiv \gamma_{\ell k}$ for $\ell \neq k$. Reassigning both the operators and the coefficients in Eq. (3.47) gives

$$\begin{aligned}\mathcal{D}^*[\bullet] = &\sum_{\ell,k} \alpha_{k\ell}\left(\Pi_k \bullet \Pi_\ell - \frac{1}{2}\{\Pi_k\Pi_\ell, \bullet\}\right) \\ &+ \sum_{k\neq\ell} \gamma_{\ell k}\left(F_{\ell k}^\dagger \bullet F_{\ell k} - \frac{1}{2}\left\{F_{\ell k}^\dagger F_{\ell k}, \bullet\right\}\right).\end{aligned} \tag{3.48}$$

We will refer to this representation as the dissipator in its thermodynamic essential form, where the first line of Eq. (3.48) is referred to as *transition* part $\mathcal{D}_F$ and the second line as the *dephasing* part $\mathcal{D}_\Pi$.
Plugging the dissipator in Eq. (3.48) into Eq. (2.80) yields the the *thermodynamic master equation*

$$\boxed{\begin{aligned}&\mathcal{L}[\rho] = -i[H_S + H_{LS}, \rho] + \\ &\Gamma\left(\sum_{\ell,k}\alpha_{k\ell}\left(\Pi_k\rho\Pi_\ell - \frac{1}{2}\{\Pi_k\Pi_\ell, \rho\}\right) + \sum_{k\neq\ell}\gamma_{\ell k}\left(F_{\ell k}\rho F_{\ell k}^\dagger - \frac{1}{2}\left\{F_{\ell k}^\dagger F_{\ell k}, \rho\right\}\right)\right).\end{aligned}} \tag{3.49}$$

It is now possible to express the coefficients $\gamma_{\ell k}$ and $\alpha_{k\ell}$ in terms of the components of the total Hamiltonians H_{SE}, H_E and H_S as defined in Eq. (2.34). By means of the relation established in Eq. (3.37) these coefficients then read

$$\gamma_{\ell k} = a_{k\ell\ell k} = \sum_{\mu,\nu} p_\nu |c_{k\nu\ell\mu}|^2 \;\; \forall \; k \neq \ell \tag{3.50}$$

and

$$\alpha_{k\ell} = a_{kk\ell\ell} = \sum_{\mu,\nu} p_\nu c_{k\nu k\mu} c^*_{\ell\nu\ell\mu}. \tag{3.51}$$

Relating these two coefficients to the elements of H_S, H_E and H_{SE} allows us to further study the implications of thermodynamic constraints like strict energy conservation (2.72) on the system dynamics. But they also allow for a deeper insight into the mathematical structure of the thermodynamic master equation given in Eq. (3.49). In Appendix E.2.3 we will be studying the properties of $\alpha_{k\ell}$, which will allow us to further simplify the structure of $\mathcal{D}$ under certain circumstances.

3.5.6 Properties of $\alpha_{k\ell}$

We will now study the properties of the coefficients $\alpha_{k\ell}$ appearing in Eq. (3.51). These coefficients constitute a matrix $(\alpha_{k\ell})$ which we will refer to as α. We now consider the complex conjugate of Eq. (3.51) and see that

$$\alpha_{k\ell}^* = \sum_{\mu,\nu} p_\nu \left(c_{k\nu k\mu} c_{\ell\nu\ell\mu}^*\right)^* = \sum_{\mu,\nu} p_\nu c_{\ell\nu\ell\mu} c_{k\nu k\mu}^* = \alpha_{\ell k}. \tag{3.52}$$

This suffices to show that $(\alpha_{k\ell}) = (\alpha_{k\ell})^\dagger$ and by that α is a Hermitian matrix. It is to be noted here that the eigenvalues p_ν of the environment thermal state τ are real and are not affected by the complex conjugate in Eq. (3.52). Additionally, for some given interaction Hamiltonians H_{SE}, α is a real symmetric matrix. One trivial example is an interaction Hamiltonian H_{SE} that only has real elements $c_{k\nu\ell\mu}$ in the eigenbasis of $H_S + H_E$. This can be directly seen when considering real coefficients in Eq. (3.52).
Two insightful qubit examples are given in Appendix C.2. Both examples employ interaction Hamiltonians with complex elements $c_{k\nu\ell\mu}$. While one of them yields a real symmetric matrix α, the other one results in a matrix α with complex components. These examples highlight that even though real symmetric H_{SE} imply real α, real α do not necessarily imply that H_{SE} is real. In Appendix E.2.3 we further investigate the effects real-valued matrices α have on the structure of the thermodynamic master equation.
The definition of $\alpha_{k\ell}$ w.r.t the elements of H_{SE} and H_E is made possible by obtaining the initial master equation from a collision model. This highlights one key advantage of the approach we took in this work – it offers more insight into the underlying structure of the coefficients appearing in the found thermodynamic master equation by linking them to the Hamiltonian in Eq. (2.34), which is the salient point of using collision models in this work.

3.5.7 Role of the Kinetic Coefficients $\gamma_{\ell k}$

In this section, we illustrate the role the kinetic coefficients $\gamma_{\ell k}$ play in the open system dynamics. We will show that these coefficients describe transitions between energy eigenstates of the system Hamiltonian H_S. In the later course of this work we will also be able to show that these transitions are related to one another by a detailed balance condition.
The first sum of the dissipator in Eq. (3.48) is comprised of transition operators $F_{k\ell}$, which motivates us to refer to it as transition part $\mathcal{D}_F$. To see how it acts on an energy eigenstate of H_S will help us to understand the role of these

kinetic coefficients.
It is to be noted here that we are dealing with the dissipator in its primal form again since we are considering the action on an actual state. To understand the role of $\mathcal{D}_F$ we will consider the action of the dissipator on an energy eigenstate of H_S with a population in the level $|j\rangle\langle j|$ and obtain

$$\begin{aligned}\mathcal{D}_F\left[|j\rangle\langle j|\right] &= \sum_{k\neq\ell}\gamma_{\ell k}\left(F_{\ell k}|j\rangle\langle j|F_{\ell k}^{\dagger}-\frac{1}{2}\left\{F_{\ell k}^{\dagger}F_{\ell k},|j\rangle\langle j|\right\}\right)\\ &= \sum_{k\neq\ell}\gamma_{\ell k}\left(|\ell\rangle\langle k|j\rangle\langle j|k\rangle\langle\ell|-\frac{1}{2}\left\{|k\rangle\langle k|,|j\rangle\langle j|\right\}\right)\\ &= \sum_{k\neq\ell}\gamma_{\ell k}\left(\delta_{kj}|\ell\rangle\langle\ell|-\frac{1}{2}\delta_{kj}\left(|k\rangle\langle j|+|j\rangle\langle k|\right)\right).\end{aligned} \tag{3.53}$$

When considering the first term in the third line of Eq. (3.53), for $k = j$, we can observe how a fixed state state $|j\rangle\langle j|$ is mapped to all the possible other states $|\ell\rangle\langle\ell|$. This happens with each respective transition rate $\gamma_{\ell j}$. The second term describes how the state is mapped to itself with a factor of $-\sum_{\ell(\neq j)}\gamma_{\ell j}$. This term sums all the transition rates from states $|j\rangle$ to $|\ell\rangle$ and recovers the state-preserving properties of the semigroup map Λ_t by keeping the action of its generator, the Lindbladian $\mathcal{L}$, traceless.
For $k \neq j$ Eq. (3.53) describes a transition from any state $|k\rangle$ other than $|j\rangle$ to $|\ell\rangle$. These transition rates vanish since all states other than $|j\rangle$ are not populated in the first place and therefore no transitions from these states can occur.
To summarise this, $\gamma_{\ell j}$ describe the transition rate from energy level $|j\rangle$ to $|\ell\rangle$. Knowing what this transition rate means will be used later when we give physical meaning to the detailed balance condition and see that it indeed describes the dynamics of an equilibration process.

3.6 Detailed Balance

In this section, we will show how a detailed balance condition can be found when employing the fact that the thermal state ρ_{th} is a fixed point of the semigroup map Λ_t. In Eq. (3.20) we proved that the thermal state ρ_{th} is the fixed point of the semigroup map Λ_t by applying the master equation following from the collision model to ρ_{th} and invoking SEC. The detailed balance condition is a ratio between the transition rates $\gamma_{\ell k}$, which can be related to the elements of the Hamiltonians found in Eq. (3.50). This connection to the Hamiltonians will render itself useful when trying to find a necessary and sufficient condition between detailed balance and strict energy conservation for exemplary sets of

Hamiltonians.

3.6.1 Employing the Fixed Point ρ_{th} of the Map Λ_t

To show that ρ_{th} is the fixed point of Λ_t we used that $\mathcal{D}[\rho_{th}] = 0$, which we proved in Eq. (3.18). We will use this vanishing action of $\mathcal{D}$ when acting on the thermal state to find that detailed balance holds for the dissipator in Eq. (3.48) and therefore also for the thermodynamic master equation in Eq. (3.49).
Since the thermal state is diagonal in the eigenbasis of H_S, we will consider the dephasing part of the dissipator acting on a single projection operator Π_i. This action can be shown to vanish by

$$\mathcal{D}_\Pi[\Pi_j] = \sum_{\ell,k} \alpha_{k\ell} \left(\Pi_k \Pi_j \Pi_\ell - \frac{1}{2} \{\Pi_k \Pi_\ell, \Pi_j\} \right) = 0, \tag{3.54}$$

since projection operators Π_j mutually commute. This result allows us to consider only the part of the dissipator that is made up of transition operators $F_{k\ell}$, namely $\mathcal{D}_F$. This reduces the vanishing action of $\mathcal{D} = \mathcal{D}_\Pi + \mathcal{D}_F$ on the thermal state to

$$\mathcal{D}[\rho_{th}] = \mathcal{D}_F[\rho_{th}] = \sum_{\ell \neq k} \gamma_{\ell k} \left(F_{\ell k} \rho_{th} F_{\ell k}^\dagger - \frac{1}{2} \left\{ F_{\ell k}^\dagger F_{\ell k}, \rho_{th} \right\} \right) = 0 \tag{3.55}$$

The transition operators $F_{k\ell}$ represent transitions between energy levels in the system Hamiltonian H_S as shown in Section 3.5.7. Therefore, they fulfil the eigenoperator condition

$$[H_S, F_{nm}] = \sum_j [\varepsilon_j |j\rangle \langle j|, |n\rangle \langle m|] = (\varepsilon_n - \varepsilon_m) |n\rangle \langle m| = -\omega_{nm} F_{nm} \tag{3.56}$$

By employing the Hadammard Lemma of the Baker Campbell Hausdorff formula $e^A B e^{-A} = \sum_{j=0}^\infty \frac{1}{j} [A, B]_j$ where $[A, B]_0 = B$ and $[A, B]_j = \Big[A, [A, B]_{j-1}\Big]$ it can be seen that

$$e^{\beta H_S} F_{nm} e^{-\beta H_S} = \sum_{j=0}^\infty \frac{1}{j!} \underbrace{[\beta H_S, F_{nm}]_j}_{(-\beta\omega_{nm})^j F_{nm}} = e^{-\beta\omega_{nm}} F_{nm}. \tag{3.57}$$

Here we used that the commutator $[\beta H_S, F_{nm}]_j$ is similar to the eigenoperator condition in Eq. (3.56) applied j-times and therefore yields $(-\beta\omega_{nm})^j$. Multiplying $e^{-\beta H_S}$ from the left to Eq. (3.57) yields the following relations for

swapping operators $e^{-\beta H_S}$ and F_{nm} and its conjugate transpose $F_{nm}^\dagger$

$$F_{nm}e^{-\beta H_S} = e^{-\beta\omega_{nm}}e^{-\beta H_S}F_{nm}, \tag{3.58}$$

$$e^{-\beta H_S}F_{nm}^\dagger = e^{-\beta\omega_{nm}}F_{nm}^\dagger e^{-\beta H_S}. \tag{3.59}$$

These results can now be employed to swap the thermal state ρ_{th} and the transition operators F_{nm} by multiplying them by a factor $e^{\pm\beta\omega_{nm}}$ to simplify the action of the dissipator to

$$\begin{aligned}\mathcal{D}\left[e^{-\beta H_S}\right] &= \sum_{\ell\neq k}\gamma_{\ell k}\left(F_{\ell k}e^{-\beta H_S}F_{\ell k}^\dagger - \frac{1}{2}\left\{F_{\ell k}^\dagger F_{\ell k}, e^{-\beta H_S}\right\}\right)\\ &= \sum_{\ell\neq k}\gamma_{\ell k}\left(e^{-\beta\omega_{\ell k}}F_{\ell k}F_{\ell k}^\dagger - F_{\ell k}^\dagger F_{\ell k}\right)e^{-\beta H_S}\\ &= \sum_{\ell\neq k}\gamma_{\ell k}\left(e^{-\beta\omega_{\ell k}}\left|\ell\right\rangle\left\langle\ell\right| - \left|k\right\rangle\left\langle k\right|\right)e^{-\beta H_S} \stackrel{!}{=} 0.\end{aligned} \tag{3.60}$$

Eq. (3.55) allows us to set the action of the dissipator in Eq. (3.60) to zero, which in turn enables us to eliminate $e^{-\beta H_S}$ by multiplying $e^{\beta H_S}$ to both sides of Eq. (3.60). As can be seen in the third line of Eq. (3.60) only diagonal elements need to be considered when evaluating the action of $\mathcal{D}$ on individual matrix elements. Evaluating this action on diagonal matrix element results in

$$\begin{aligned}\left\langle i\right|\mathcal{D}\left[e^{-\beta H_S}\right]\left|i\right\rangle &= \sum_{k(\neq i)}\gamma_{ik}e^{-\beta\omega_{ik}} - \sum_{\ell(\neq i)}\gamma_{\ell i}\\ &= \sum_{k(\neq i)}\left(\gamma_{ik}e^{-\beta\omega_{ik}} - \gamma_{ki}\right) \stackrel{!}{=} 0.\end{aligned} \tag{3.61}$$

Eq. (3.61) constitutes a set of d_S equations that are each set to zero due to Eq. (3.55). It can be seen that these equations can be solved by setting each term $\gamma_{ik}e^{-\beta\omega_{ik}} - \gamma_{ki}$ in the sum to zero individually. Rearranging these terms then yields the following solutions to these equations

$$\frac{\gamma_{\ell k}}{\gamma_{k\ell}} = e^{\beta\omega_{\ell k}} \qquad \forall\gamma_{k\ell}\neq 0,\ \ell < k. \tag{3.62}$$

These solutions are the desired detailed balance condition between energy levels $\left|\ell\right\rangle$ and $\left|k\right\rangle$ of the system Hamiltonian H_S and represent a central result of this work. The detailed balance conditions sets the before found transition rates $\gamma_{\ell k}$ into a ratio and relates them to the Bohr frequencies. To avoid redundant equations we demanded $\ell < k$ in Eq. (3.62) and also in the following derivations.

3.6.2 Physical Interpretation of Detailed Balance

To give more meaning to Eq. (3.62) we focus on what this detailed balance condition tells us about the population of the energy levels of the system Hamiltonian. Therefore, we will consider the case where energy level $|k\rangle$ has higher energy than level $|\ell\rangle$, i.e. $\varepsilon_k > \varepsilon_\ell$. Rearranging Eq. (3.62) reveals that

$$\gamma_{\ell k} = \gamma_{k\ell} e^{\beta(\varepsilon_k - \varepsilon_l)} > \gamma_{kl} \qquad \forall\ \varepsilon_k > \varepsilon_l, \beta > 0. \tag{3.63}$$

The transition rate $\gamma_{\ell k}$, describing the transition from energy levels $|k\rangle$ to $|\ell\rangle$, is higher than the opposing transition rate $\gamma_{k\ell}$ if energies $\varepsilon_k > \varepsilon_l$. Therefore, the detailed balance condition in Eq. (3.62) describes the behaviour of an equilibration process where a system equilibrates with its environment since it makes a population of the lower energy levels more likely than the higher ones. This behaviour also meets our expectations due to our day-to-day experiences, where hot objects cool down until they reach the temperature of their colder environment.

3.6.3 Inner Structure of the Detailed Balance Condition

Detailed balance as in Eq. (3.62) obscures the inner structure of the transition rates $\gamma_{\ell k}$. With the help of the results of Eq. (3.50), which are a direct consequence of an energy-conserving collision model, it is possible to find a detailed balance condition that depends only on elements of the set of Hamiltonians in Eq. (2.34). Plugging in these results reveals the detailed balance condition

$$\boxed{\frac{\gamma_{k\ell}}{\gamma_{\ell k}} = \frac{\sum\limits_{\mu,\nu} p_\nu \left|c_{\ell\nu k\mu}\right|^2}{\sum\limits_{\alpha,\beta} p_\beta \left|c_{k\beta\ell\alpha}\right|^2} = e^{\beta\omega_{k\ell}} \qquad \forall\ k \neq \ell.} \tag{3.64}$$

This connection between the detailed balance condition and the coefficients of the Hamiltonians allows for constructing these Hamiltonians from a given DB compliant master equation. This construction will then in turn allow for checking if SEC is also fulfilled. This analysis is possible since we found a master equation following from a collision model and therefore enables us to find out more about the underlying relation between SEC and DB.

3.7 Detailed Balance Compliant Master Equation and Strict Energy Conservation

Following the course of this work so far, we see that a strict energy-conserving collision model leads to a detailed balance for non-degenerate Bohr-frequencies $\omega_{\ell k}$. It is a priori unclear if a detailed balance-compliant master equation also implies the existence of an underlying total Hamiltonian that satisfies strict energy conservation. In this section, we will construct Hamiltonians from a DB compliant master equation and show that it is possible to construct at least two that also fulfil SEC for each dimension $d_S = d_E$.
This construction is based on the kinetic coefficients $\gamma_{\ell k}$, the eigenenergies ε_i of the system Hamiltonian H_S and the eigenvalues $p_\nu = e^{-\beta\epsilon_\nu}/Z_E$ of the environment thermal state τ appearing in the detailed balance condition (c.f. Eq. (3.64))

$$\frac{\gamma_{k\ell}}{\gamma_{\ell k}} = \frac{\sum\limits_{\mu,\nu} p_\nu \left|c_{\ell\nu k\mu}\right|^2}{\sum\limits_{\alpha,\beta} p_\beta \left|c_{k\beta\ell\alpha}\right|^2} = e^{\beta\omega_{k\ell}} \qquad \forall\ k \neq \ell,$$

and the thermodynamically essential form of the master equation (c.f. Eq. (3.49))

$$\mathcal{L}[\rho] = -i\left[H_S + H_{LS}, \rho\right] + \Gamma\left(\sum_{\ell,k} \alpha_{k\ell}\left(\Pi_k \rho \Pi_\ell - \frac{1}{2}\left\{\Pi_k\Pi_\ell, \rho\right\}\right) + \sum_{k\neq\ell} \gamma_{\ell k}\left(F_{\ell k}\rho F_{\ell k}^\dagger - \frac{1}{2}\left\{F_{\ell k}^\dagger F_{\ell k}, \rho\right\}\right)\right).$$

These coefficients are then used to construct the individual terms of the Hamiltonian $H = H_S + H_E + H_{SE}$, where

$$H_S = \sum_i \varepsilon_i \left|i\right\rangle\left\langle i\right|,\ H_E = \sum_\gamma \epsilon_\gamma \left|\gamma\right\rangle\left\langle\gamma\right|,\ H_{SE} = g\sum_{i,j,\mu,\nu} c_{i\mu j\nu}\left|i\right\rangle\left\langle j\right| \otimes \left|\mu\right\rangle\left\langle\nu\right|. \tag{3.65}$$

In the following example we show, that with a single given master equation following from a DB compliant collision model, one can construct non-unique sets of Hamiltonians that yield said master equation via a CM, where one fulfils SEC and one doesn't. This construction is based on the master equations kinetic coefficients γ_{kl}, fulfilling Eq. (3.64). Therefore, all of the found Hamiltonians are compliant with detailed balance, but only some of them also fulfil strict energy conservation. This already points out that whether or not energy conservation is also fulfilled depends on the construction.

3.7.1 Qubit Examples of Detailed Balance Compliant Master Equations

We will now derive a set of Hamiltonians from a given master equation in $dS = dE = 2$ resulting from a collision model that we demand to fulfil detailed balance. For an inverse temperature $\beta = 1$ we are given the kinetic coefficients

$$\gamma_{01} = 2,\ \gamma_{10} = 1. \tag{3.66}$$

From this statement of parameters, we can construct a set of Hamiltonians that has to fulfil Eq. (3.64), since we know (γ) and (α) defined by Eqs. (3.50) and (3.51) from its origin of the collision model. We start by computing the Bohr frequency $\omega_{01} = \varepsilon_1 - \varepsilon_0$ in terms of the eigenenergies of the system H_S. Without loss of generality we set the first eigenenergy $\varepsilon_0 = 0$ and by employing $\frac{\gamma_{01}}{\gamma_{10}} = e^{\beta\omega_{01}}$ we construct H_S. The detailed balance condition doesn't strictly restrict the structure of V, it can be chosen freely. However there is a relation between V's elements $c_{k\mu l\nu}$ and the eigenenergies p_ν of the thermal state τ which depends on the environment free Hamiltonian H_E due to DB in Eq. (3.64). In this case, we chose V to be anti-diagonal and solving detailed balance in Eq. (3.62) for $\frac{p_\nu}{p_\mu}$ allows for a construction of H_E. This construction results in the Hamiltonians

$$H_S = \begin{pmatrix} 0 & 0 \\ 0 & \log(2) \end{pmatrix} \quad V \stackrel{!}{=} \begin{pmatrix} 0 & 0 & 0 & 3 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 3 & 0 & 0 & 0 \end{pmatrix} \quad H_E = \begin{pmatrix} 1 & 0 \\ 0 & -\log(5) \end{pmatrix}. \tag{3.67}$$

It is important to note here that this construction is not unique but it complies with the detailed detailed balance condition in Eq. (3.64) and follows from the given kinetic coefficients given in Eq. (3.66) at inverse temperature $\beta = 1$.
Computing the commutator for strict energy conservation in Eq. (2.72) then results in

$$g\left[V, H_S + H_E\right] = g \begin{pmatrix} 0 & 0 & 0 & -3\log\left(\frac{5}{2}\right) \\ 0 & 0 & \log(10) & 0 \\ 0 & -\log(10) & 0 & 0 \\ \log\left(\frac{125}{8}\right) & 0 & 0 & 0 \end{pmatrix} \neq 0. \tag{3.68}$$

Therefore, we immediately see that strict energy conservation is not necessarily a direct consequence of detailed balance. However, another construction based on the same master equation defined by its kinetic coefficients in Eq. (3.66)

and at the same inverse temperature $\beta = 1$ leads to a different result. Here the ratio $\frac{\gamma_{01}}{\gamma_{10}}$ leads to the same H_S but by a different choice of V we find a different H_E. Summarized, this construction reads

$$H_S = \begin{pmatrix} 0 & 0 \\ 0 & \log(2) \end{pmatrix} \quad V \stackrel{!}{=} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} \quad H_E = \begin{pmatrix} 0 & 0 \\ 0 & \log(2) \end{pmatrix}. \tag{3.69}$$

For this choice of V we find that the energy gaps in the system's and the environment's free Hamiltonians need to be the same for detailed balance as in Eq. (3.64) to be fulfilled. Computing the commutator (Eq. (2.72)) for the Hamiltonians in Eq. (3.69) results in

$$g\left[V, H_S + H_E\right] = 0, \tag{3.70}$$

which shows that strict energy conservation is fulfilled as well. A similar reasoning to why $g \to \infty$ multiplied by zero still results in zero as we have explained in Eq. (2.58) applies here.
For both of these qubit examples, the Lamb shift Hamiltonian H_{LS} (Eq. (2.70)) vanishes. The factor g, approaching in infinity in the continuous time limit also scales the Lamb shift but isn't met by a infinitesimal Δt here. In both cases

$$H_{LS} = \mathrm{tr}_E\left(H_{SE}\tau\right) = g\mathrm{tr}_E\left(V\tau\right) = 0, \tag{3.71}$$

since the partial trace vanishes.

3.7.2 Construction of Sparsely Populated Interaction Hamiltonians in Higher Dimensions

Nevertheless, we are able to show that there exists always at least one construction of Hamiltonians from a DB compliant master equation which also fulfils SEC for $d_S = d_E$. Showing that each detailed balance-compliant master equation might have come from a strict energy-conserving total Hamiltonian, even if the underlying structure of the master equation isn't uniquely defined. For any given master equation that follows from a collision model, we immediately know all the factors $\gamma_{k\ell}$ and $\alpha_{k\ell}$ by Eqs. (3.50) and (3.51). In these equations, it can be seen that the coefficients α_{ij} are composed of elements of the interaction Hamiltonian $c_{k\mu\ell\nu}$ for $k = \ell$. The coefficients $\gamma_{k\ell}$ are exactly

those where $k \neq \ell$. This means that the coefficients $\gamma_{k\ell}$ and $\alpha_{k\ell}$ address different parts of H_{SE} and are therefore independent of each other. Additionally, since the coefficients $\alpha_{k\ell}$ do not appear in the detailed balance condition in Eq. (3.64), we do not have to explicitly consider them in this construction and focus only on the part of the master equation scaled by the coefficients $\gamma_{k\ell}$.
By rearranging the detailed balance condition (Eq. (3.62)) we find the Bohr frequencies

$$\omega_{\ell k} = \frac{1}{\beta} \ln\left(\frac{\gamma_{\ell k}}{\gamma_{k\ell}}\right) = \varepsilon_k - \varepsilon_\ell, \tag{3.72}$$

of the system Hamiltonian H_S in relation to the ratio of kinetic coefficients $\gamma_{\ell k}$. By fixing one eigenenergy ε_ℓ of H_S, all the other eigenenergies can be defined by the energy gaps (Bohr frequencies $\omega_{\ell k}$) relative to the fixed one. This restriction also points out that not all $\gamma_{\ell k}$ in a master equation that fulfils detailed balance can be chosen freely. However, together with these constraints knowing the coefficients $\gamma_{\ell k}$ allows for defining the entire system Hamiltonian H_S up to a constant phase, i.e.

$$H_S' = H_S + x\mathbb{1}_S \qquad \forall x \in \mathbb{R}. \tag{3.73}$$

While the energy gaps of H_S are fixed through detailed balance, the construction of V and H_E offers some leeway. For simplicity, we are assuming that the interaction Hamiltonians V is sparsely populated. By a sparsely populated Hamiltonian we mean that in each off-diagonal block (k, ℓ) for $k \neq \ell$ there is exactly one non-vanishing element $c_{k\mu\ell\nu}$. Its conjugate transpose $c_{\ell\nu k\mu} = c^*_{k\mu\ell\nu}$ populates the block (ℓ, k). The diagonal blocks (k, ℓ) for $k = \ell$ are assumed to be empty in these sparsely populated Hamiltonians V. For qubits where $d_S = d_E = 2$ there are exactly two elements that are non-vanishing in a sparsely populated interaction Hamiltonian. One element is in the Block $(k, \ell) = (1, 0)$ and the other one in the block $(k, \ell) = (1, 0)$, e.g.

$$V = \sum_{k,\ell=0}^{1} \sum_{\mu,\nu=0}^{1} c_{k\mu\ell\nu} \left|k\mu\right\rangle \left\langle\ell\nu\right| = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & c_{0110} & 0 \\ 0 & c_{1001} & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{3.74}$$

Additionally to V being sparsely populated, we demand that the indices of the non-vanishing $c_{k\mu\ell\nu}$ in the system and environmental degrees of freedom coincide such that $\delta_{\ell\mu}$ and $\delta_{k\nu}$ describe which elements vanish in the off-diagonal

block. The interaction Hamiltonian then reads

$$V = \sum_{k\neq\ell} \sum_{\mu,\nu} c_{k\mu\ell\nu}\delta_{\ell\mu}\delta_{k\nu} \left|k\mu\right\rangle \left\langle \ell\nu\right| \tag{3.75}$$

Computing detailed balance as defined in Eq. (3.64) for our chosen H_S and sparsely populated V then results in

$$\frac{\gamma_{k\ell}}{\gamma_{\ell k}} = \frac{\sum\limits_{\mu,\nu} p_\nu \left|c_{\ell\nu k\mu}\right|^2}{\sum\limits_{\alpha,\beta} p_\alpha \left|c_{k\alpha\ell\beta}\right|^2} = \frac{p_\nu \left|c_{\ell\nu k\mu}\right|^2 \delta_{\ell\mu}\delta_{k\nu}}{p_\mu \left|c_{k\mu\ell\nu}\right|^2 \delta_{\ell\mu}\delta_{k\nu}} = \frac{p_k}{p_\ell} = e^{-\beta(\epsilon_k-\epsilon_\ell)} = e^{\beta(\varepsilon_\ell-\varepsilon_k)}. \tag{3.76}$$

Here we used that $c_{k\mu\ell\nu} = c^*_{\ell\nu k\mu}$ and therefore, their absolute values cancel. Additionally, we plugged in $p_\nu = e^{-\beta\epsilon_\nu}$, the eigenvalues of τ. The last equality follows directly from detailed balance in Eq. (3.62) and plugging in the eigenenergies of H_S into the Bohr frequency $\omega_{k\ell} = \varepsilon_\ell - \varepsilon_k$.
Therefore, detailed balance with our choice of a sparsely populated V demands that

$$\epsilon_\ell - \epsilon_k = \varepsilon_\ell - \varepsilon_k \tag{3.77}$$

Which means that by restricting H_{SE} with $\delta_{\ell\mu}$ and $\delta_{k\nu}$ we also demand that the energy gaps in system $(\varepsilon_\ell - \varepsilon_k)$ and environment $(\epsilon_\ell - \epsilon_k)$ are equivalent. This result allows us to construct the environment Hamiltonian such that

$$H'_E = H_E + y\mathbb{1}_E \qquad \forall y \in \mathbb{R}, \tag{3.78}$$

where we choose y such that the eigenenergies of H_E exactly coincide with the ones of H_S.
This set of Hamiltonians

$$H_S = \sum_{k=0}^{d_S-1} \varepsilon_k \left|k\right\rangle \left\langle k\right| \quad H_E = \sum_{\nu=0}^{d_E-1} \varepsilon_\nu \left|\nu\right\rangle \left\langle \nu\right| \quad V = \sum_{k\neq\ell} \sum_{\mu,\nu} c_{k\mu\ell\nu}\delta_{\ell\mu}\delta_{k\nu} \left|k\mu\right\rangle \left\langle \ell\nu\right| \tag{3.79}$$

follows from a master equation where we know that its kinetic coefficients fulfil DB. Computing the commutator given in Eq. (2.72) results in

$$\begin{aligned} &g\left[H_S + H_E, V\right] = \\ &= g\left[\sum_{k=0}^{d_S-1} \varepsilon_j \left|j\right\rangle \left\langle j\right| + \sum_{\chi=0}^{d_E-1} \varepsilon_\chi \left|\chi\right\rangle \left\langle \chi\right|, \sum_{k\neq\ell} \sum_{\mu,\nu} c_{k\mu\ell\nu}\delta_{\ell\mu}\delta_{k\nu} \left|k\mu\right\rangle \left\langle \ell\nu\right|\right] \\ &= g \sum_{k\neq\ell} c_{k\ell\ell k} \left|k\ell\right\rangle \left\langle \ell k\right| (\varepsilon_k + \varepsilon_\ell - \varepsilon_\ell - \varepsilon_k) = 0, \end{aligned} \tag{3.80}$$

which shows that we found a set of Hamiltonians that also fulfils SEC. It is to note here that we scale g such that when multiplied with $\Delta t \to 0$ in the continuous time limit (see Section 2.2.3) it approaches a finite constant $\Gamma = g^2 \Delta t$. It does approach infinity but when multiplied with a number that approaches zero in the same limit it results in a finite value. Therefore, the vanishing commutator in Eq. (3.80) multiplied with g vanishes as well, similar as in Eq. (2.58).

With these assumptions, it is always possible to construct Hamiltonians from a master equation with kinetic coefficients $\gamma_{\ell k}$ that fulfil DB that then also fulfil SEC for all $d_S = d_E$. Additionally, for a choice of a sparsely populated V, where only the elements $c_{k\mu\ell\nu}\delta_{k\mu}$ and $c_{k\mu\ell\nu}\delta_{\ell\nu}$ for $k \neq \ell$ are populated, we find that the energy gaps in H_E need negative to those of H_S to fulfil DB. This construction then also fulfils SEC. Therefore, from a given master equation that fulfils detailed balance and follows from a collision model, we can always construct at least two sets of Hamiltonians that then also fulfil strict energy conservation. This result hints that wherever the DB compliant master equation came from, it might have always come from an energy-conserving system. In other words, any detailed balance condition following from a collision model can always be traced back to a setup based on a strict energy-conserving Hamiltonian.

However, these two solutions are certainly not the only possible constructions of H following from a DB compliant ME. In the next section, we present a construction method for all sparsely populated V that are compliant with DB for arbitrary dimensions $d_S = d_E$.

3.7.3 General Construction Methods for Higher Dimensions

In this Section, we construct sets of Hamiltonians (H_S, H_E, H_{SE}) that are compliant with detailed balance and follow from a collision model. In that sense, they are defined by their kinetic coefficients $\gamma_{\ell k}$, that fulfil detailed balance as in Eq. (3.64). We present a calculation that constructs all detailed balance-compliant sets of Hamiltonians for arbitrary dimensions $d_S = d_E$ and sparsely populated interaction Hamiltonians $H_{SE} = gV$. For each of these results, it is then possible to compute the commutation relation in Eq. (2.72) which determines if the resulting set of Hamiltonians also fulfils strict energy conservation. The instructions in this Section are supplementary to the Mathematica notebook in Appendix D.1.

Similarly to the construction in Section 3.7, H_S' and H_S in Eq. (3.73) lead to the same free dynamics according to the unitary evolution and have the same Bohr frequencies ω_{kl}. This shift allows for a free choice of constructing

the system Hamiltonian H_S by employing the given coefficients $\gamma_{\ell k}$. For this calculation, we choose to set the first eigenenergy $\varepsilon_0 = 0$ and compute all the other eigenenergies relative to ε_0 according to Eq. (3.72). This calculation constructs the system Hamiltonian

$$H_S = \mathrm{diag}(\varepsilon_0, \varepsilon_1, \ldots, \varepsilon_{d_S-1}) = \frac{1}{\beta}\mathrm{diag}\left(0, \ln\left(\frac{\gamma_{01}}{\gamma_{10}}\right), \ldots, \ln\left(\frac{\gamma_{0(d_S-1)}}{\gamma_{(d_S-1)0}}\right)\right). \tag{3.81}$$

This choice of a system Hamiltonian is only unique up to a constant phase that can be added without changing the dynamics of the open quantum system.
We then continue to construct H_E and V relative to H_S. We again choose V to be sparsely populated such that only one element in the sum in Eq. (3.64) contributes. This lets us find a relation for the energy gaps of the system $(\varepsilon_k - \varepsilon_\ell)$ and environment $(\epsilon_\nu - \epsilon_\mu)$ Hamiltonians are related in the following way

$$\epsilon_\nu - \epsilon_\mu = \varepsilon_k - \varepsilon_\ell. \tag{3.82}$$

Here, the indices k, ℓ, μ, ν depend on the specific population in the interaction Hamiltonian.
We now illustrate the working principle of the calculation in Appendix D.1 based on an example in $d_S = d_E = 3$. First, we fix the system indices (k, ℓ) and compute all possible variations of (ν, μ) which we refer to the arrays `kls` and `numus` in the Mathematica NB. In the detailed balance condition in Eq. (3.62) each index pair (k, ℓ) appears also swapped in $\frac{\gamma_{k\ell}}{\gamma_{\ell k}}$, therefore we additionally require $k > \ell$ to avoid redundant index combinations. On the other hand, some of the index combinations (ν, μ) are not compliant with detailed balance. For these index pairs, Eq. (3.82) can't be solved and they are excluded from further calculations. However, if these sets of equations can be solved then the indices (ν, μ) are considered for the construction of the Hamiltonians V and H_E.
We illustrate how these equations are solved on hand of an example where the fixed choice of indices is `kls` $= \{\{0,1\},\{0,2\},\{1,2\}\}$ and one detailed balance compliant rotation is `numus` $= \{\{0,2\},\{0,1\},\{2,1\}\}$. These index combinations applied to Eq. (3.82) result in the set of equations

$$\begin{aligned} \varepsilon_0 - \varepsilon_1 &= \epsilon_0 - \epsilon_2 \\ \varepsilon_0 - \varepsilon_2 &= \epsilon_0 - \epsilon_1 \\ \varepsilon_1 - \varepsilon_2 &= \epsilon_2 - \epsilon_1. \end{aligned} \tag{3.83}$$

Similarly to the system Hamiltonian in Eq. (3.81) where we set $\varepsilon_0 = 0$, we will also set the first eigenenergy of the environment Hamiltonian $\epsilon_0 = 0$. Again

we are only interested in energy gaps and not what the actual eigenenergies of H_S and H_E are. Solving the equations in Eq. (3.83) for the eigenenergies ϵ_ν of H_E results in

$$\epsilon_0 = 0 \qquad \epsilon_1 = \varepsilon_2 \qquad \epsilon_2 = \varepsilon_1 \tag{3.84}$$

Since the set of equations in Eq. (3.83) is solvable the chosen pairs of (k, ℓ) and (ν, μ) fulfil detailed balance and we can populate the coefficients $c_{k\mu\ell\nu}$ of the interaction Hamiltonian V according to Eq. (3.64) and find a set of Hamiltonians

$$H_S = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \varepsilon_1 & 0 \\ 0 & 0 & \varepsilon_2 \end{pmatrix}, \; H_E = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \varepsilon_2 & 0 \\ 0 & 0 & \varepsilon_1 \end{pmatrix},$$

$$V = \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & c_{0,1,2,0} & 0 & 0 \\ 0 & 0 & 0 & c_{0,2,1,0} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & (c_{0,2,1,0})^* & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & c_{1,1,2,2} \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & (c_{0,1,2,0})^* & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & (c_{1,1,2,2})^* & 0 & 0 & 0 & 0 \end{pmatrix} \tag{3.85}$$

For each of these sets of Hamiltonians (H_S, H_E, H_{SE}) that directly follow from a master equation that fulfils detailed balance we can compute the commutator in Eq. (2.72). The resulting set in Eq. (3.85) fulfils the commutation relation

$$g\,[V, H_S + H_E] = 0, \tag{3.86}$$

and we see that also SEC holds for this example.

The Mathematica NB in Appendix D.1 was used to compute all sparsely populated interactions Hamiltonians V for dimensions $d_S = d_E = (2, 3, 4)$ that follow from a detailed balance compliant master equation. We found that for each resulting set of Hamiltonians, strict energy conservation also holds. To avoid diverging unitary behaviour we also confirmed that the Lamb shift vanishes for each individual set of Hamiltonians. This Mathematica NB could in principle be used for arbitrary dimensions $d_S = d_E$. However, the number of possible combinations (ν, μ) scales in a factorial manner and for $d_E > 4$ the table `numus` can't be computed by a laptop computer with 16 GB of RAM.

We can now conclude that for at least 2, 3 and 4 dimensions all constrictions of H_S, H_E and sparsely populated V, constructed from the detailed balance compliant $\gamma_{\ell k}$ of a master equation following from a collision model, also fulfil strict energy conservation.
Since these results come at great computational cost and don't allow for calculations in dimensions greater than $d_S = d_E = 4$ on a regular laptop computer we give an outlook on how this calculation could be made more efficient in Section 5.1.

4 Discussion

In the approach we used in this work, most of the assumptions are implemented directly in the setup of the collision model. The first major assumption we made was that the open system dynamics are modelled by a Markovian collision model. Therefore, we assumed how the open system interacts with the environment and about the environment itself. These major simplifications result in a quantum master equation of GKSL form by additionally taking the continuous-time limit. In Section 4.2.1 we will take account of a similar Markovian CM setup where this limit is taken in a coarse-graining approach. By setting up the CM such that the system dynamics follow basic thermodynamic assumptions we were able to further restrict the dynamic description of the open quantum system. To get to these results the thermodynamic assumptions were implemented by demanding that strict energy conservation holds and that the environment is in a thermal equilibrium state.
In this approach we were able to reproduce the structure of a thermodynamically informed GKSL equation of Dann and Kosloff [4], despite following a different path. We will, therefore start this discussion by giving an account of the differences and similarities between our work and the results of Ref. [4].

4.1 Comparing our Results to Existing Results in the Literature

4.1.1 Dann and Kosloff's Approach

Dann and Kosloff [4] employed an approach to implement thermodynamic assumptions to an existing GKSL equation that is formulated in an axiomatic way based on five thermodynamically informed postulates. We have recited these postulates in the following list and compared them to the approach we took:

- **Postulate 1**: " *The dynamical map is a completely positive trace-preserving (CPTP).*"
  The dynamical map is used to describe the dynamic evolution directly. The individual collisions in our approach are also described by a dynamical map that is CPTP. However, we go on and find a dynamical description based on the semigroup map, that we use to determine which elements of the master equation contribute to the overall dynamics.

- **Postulate 2**: " *The environment is initially in a stationary state with respect to the environment's free Hamiltonian $\hat{H}_E$. In the thermodynamic limit, we can extend this condition to all times.*"

By assuming that the environment is in a thermal equilibrium state, the thermal state τ, we directly imply that it is stationary with its free Hamiltonian H_E. In the setup of the CM we additionally assumed that the environment states that have not interacted with the system yet are uncorrelated to it. Therefore, for each future interaction the environment states are still stationary w.r.t. their free Hamiltonian H_E.

- **Postulate 3**: "*The fixed point of the dynamical map is a thermal state.*"
  We did not need to make this assumption, since we were able to show that the thermal state ρ_{th} is the fixed point of the semigroup map Λ_t in Eq. (3.20).

- **Postulate 4**: "*The dynamical map Λ_t is Markovian.*"
  We also assumed that the open system dynamics are Markovian. However, we derive a master equation based on the interactions in a collision model employing a dynamical map, while the authors of Ref. [4] set this map to be equivalent to the semigroup map Λ_t. In Appendix B.1 we show in an example that these two maps do not necessarily lead to the same dynamics and directly equating them is at least an additional assumption that we do not have to make.

- **Postulate 5**: "*Strict energy conservation.*"
  The individual collisions are modelled by a dynamical map, where the unitary transformation of the composite $S - E$ fulfils SEC.

Despite some of our assumptions differ we were able to reproduce the results they found, like the final form of the master equation master equation in its thermodynamic essential form, as well as detailed balance. Additionally, our approach gives a direct connection between the original system-environment dynamics and the resulting master equation, which is useful for deriving conditions where a detailed balance-compliant master equation directly leads to strict energy conservation. To illustrate the differences and similarities in the respective approaches to deriving thermodynamically compliant master equations, we have given an overview in Figures 4.1 and 4.2.

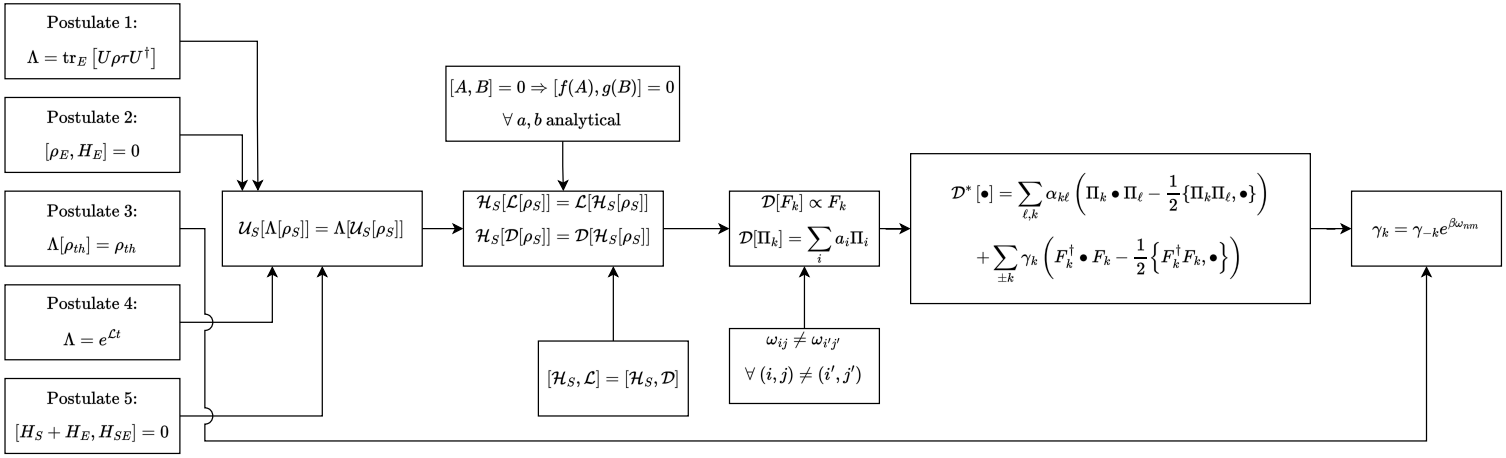


Figure 4.1: Approach taken in the work of Dann and Kosloff [4]

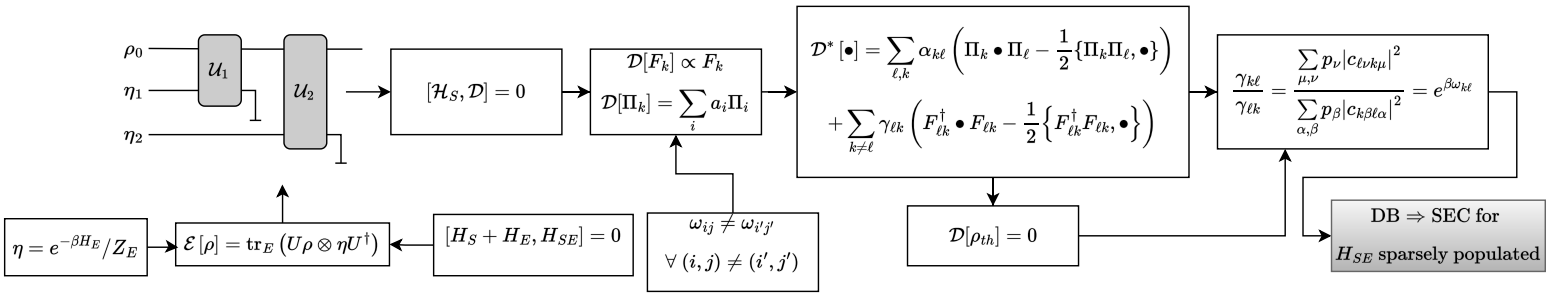


Figure 4.2: Approach taken in this work

4.1.2 Detailed Balance in Open Quantum Systems

Detailed balance is deeply linked to equilibrium and was found for several OQS setups. It was presented following a microscopic approach by Breuer and Pettrucione [7] where we compared their result directly to ours in Appendix B.2.
In Ciccarello [30] they also found a detailed balance condition for open system dynamics. Since they considered a quantum optics setup it can't be compared directly to us but shows a similar relation between SEC and DB as the one we found. Dümcke [10] found detailed balance following from energy conservation in a Bose and a Fermi gas by modelling successive collisions.

4.2 Collision Models and their Physical Meaning

In this work, we have seen that thermodynamic properties can be implemented into a collision model by demanding that the interaction between the system and environment follows strict energy conservation while the environment remains in a thermal equilibrium state. While this implementation was straightforward in mathematical terms, we want to give an account of the physical meaning of collision models in general.
Collision models have to be considered theoretical toy models. Even though they do find their experimental counterparts in e.g. the experimental realisation of a micromaser [14], where the open system dynamics of a lossy cavity mode can be described by a collision model [11–13]. Describing the setup at hand by a Markovian CM is justified by assuming that the atoms, in the beam entering the cavity, are themselves non-interacting and are initially uncorrelated.
To summarize, CMs offer a theoretical description of conceptual issues in open quantum systems theory that might not be solvable with different approaches and have proven their validity in experimental realisations. Especially non-Markovian dynamics might get tedious in the microscopic approach by introducing tools like a Memory Kernel [7]. Non-Markovian Collision models offer a more straigth forward approach to introducing memory as we sketch in an outlook in Section 5.2.

4.2.1 Modelling of Time Steps

In the continuous-time limit, we assumed that the product $\Gamma = g^2\Delta t$ is finite in the limit of $\Delta t \to 0$, while $g \to \infty$ at the same time. However, the coefficient g still appears in the Lamb shift term $H_{LS} = \mathrm{tr}_E(gV\tau)$ of the master

equation (2.65), which would in turn also approach infinity and outweigh the dissipative part of the ME. In Ref. [16], it is argued that usually, the average of the Lamb shift term vanishes or that a renormalization of the free system Hamiltonian H_S is applied to avoid divergent behaviour.
To avoid problems with diverging terms in our master equation we made similar assumptions as in Ref. [16] and for all our examples in the Appendix, we chose Hamiltonians for which H_{LS} vanishes, before taking the limit of $g \to \infty$. However, this certainly is not always the case [44] and we might as well have constructed H_{LS} such that we find energy-conserving Hamiltonians that follow from a detailed balance-compliant collision model that would require renormalization of the unitary terms of the master equation. For such cases, different construction methods as in Ref. [30] might be advantageous, where they applied the continuous-time limit via coarse graining of timesteps. This approach results in a dissipator where the dynamic evolution depends on the chosen time step length. These steps have to be chosen carefully since for ever shorter time step length the action of the dissipator vanishes and the dynamics become unitary. However, there is no explicit dependency on time step length or interaction strength in the unitary part of the resulting master equation and therefore also no divergent behaviour of the the Lamb shift terms. This approach is probably more suitable to simulate open system dynamics in discrete numerical simulations where the time step length can be chosen as a simulation parameter.

5 Outlook

5.1 Extending the Set of Hamilonians Compliant with Detailed Balance

In Section 3.7 we have shown that for every dimension $d_S = d_E$ there are at least two possible constructions of Hamiltonians following from the kinetic coefficients $\gamma_{\ell k}$, that fulfil detailed balance according to Eq. (3.64). These are exactly those Hamiltonians where the energy gaps in H_S and H_E are either equivalent or opposite and the interaction is governed by a sparsely populated V. In Section 3.7.3 we have shown how to compute additional sets of Hamiltonians from the same properties. However, this construction is computationally intensive and we were not able to compute these sets for dimensions larger than $d_S = d_E = 4$ on a regular laptop computer. Therefore, we present an outlook on how this calculation could be made more efficient.

5.1.1 Decrease RAM Usage by Discarding non-DB Compliant Equations

In the calculation presented in Section 3.7.3, for each dimension the number of solvable equations is much smaller than the total number of combinations possible for fixed (k, l). While in three dimensions out of the 48 total combinations, only 12 are solvable, in four dimensions it's only 48 out of 46080. This shows a huge potential in reducing the need for RAM in the computation. Solving the set of equations following from Eq. (3.82) directly after the pairs are created individually allows for discarding the unsolvable combinations right away. However, at some point, this calculation will become unfeasible again and is not suitable to find all sparsely populated Hamiltionians V following from a DB compliant ME in even higher dimensions.

5.1.2 Combinatorics Approach

A possible step to make the numerical computation obsolete is to detect patterns in the solvable equations following from Eq. (3.82) and infer how the index combinations in higher dimensions might look. The following notes can give an idea of how this works based on examples in $d_S = d_E = 3$ for $\texttt{kls} = ((0,1),(0,2),(1,2))$

- equal and opposite energy gaps are always a solution:
  $\texttt{numus} = ((0,1),(0,2),(1,2))$ and $\texttt{numus} = ((1,0),(2,0),(2,1))$

- for each found solution, swapping the indices in the individual (ν, μ) is also a solution.
- the reverse order of pairs that form a solution is always a solution: $\texttt{numus} = ((0,1),(0,2),(1,2)) \Rightarrow \texttt{numus} = ((1,2),(0,2),(0,1))$

Just detecting patterns certainly does not hold for a general derivation of all possible constructions. However, understanding how these constructions come about might give an idea of the underlying connection between detailed balance and strict energy conservation.

5.1.3 Dimensions $d_S \neq d_E$ and Degenerate Ratios $\gamma_{\ell k}/\gamma_{k\ell}$

We have only constructed sets of Hamiltonians for dimensions $d_S = d_E$ so far. Considering non-matching dimensions will certainly lead to some kind of degeneracies in the spectra of the system's and environment's free Hamiltonians and possibly also in the ratios $\gamma_{\ell k}/\gamma_{k\ell}$. Following the approach taken in this work, we find DB by applying a ME resulting from a thermodynamic collision model to its fixed point. To find this master equation we had to assume that the Bohr frequencies $\omega_{\ell k}$ of H_S are non-degenerate. This also implies that the eigenenergies of the system are non-degenerate. It is unclear how a possible degeneracy in the eigenenergies will affect the results. When the non-invariant spectrum composed of transition operators $F_{k\ell}$ experiences degeneracies, the eigenoperators of the dissipator $\mathcal{D}$ are represented by a linear combination of the degenerate transition operators $\{F_{nm}\}$. However, in Ref. [4] an outlook is given of how these degeneracies might influence the structure of the dissipator in a way that it may include cross terms of F_{nm}'s. The implications of degeneracies in the ratios $\gamma_{\ell k}/\gamma_{k\ell}$ that directly lead to degenerate Bohr-frequencies are unclear and require further investigation.

5.2 Non-Markovian Dynamics

A CM setup is a perfectly suitable approach to implement memory to a given model. Here, we introduce one method to implement memory based on the work of Kretschmer et al. [45]. Their proposed collision model includes ancilla–ancilla collisions after each ancilla collision with the system. It is reasonable to assume that these interactions in the environment happen as these collisions can also occur in principle. These memory effects are modelled by including another unitary interaction of the environment state after interaction with the system with a fresh environment state η. This interaction is represented by $\mathcal{V}_1$ in Figure 5.1.

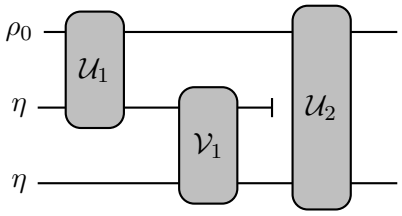


Figure 5.1: Non-Markovian collision model portraying the first two interactions of the system with its environment. The system's initial state ρ_0 interacts with its initially uncorrelated environment (η) followed by an interaction with the now correlated ancilla.

By allowing for these ancilla-ancilla interactions the interaction between the ancillas could be modelled in a unitary fashion and was scaled with a real-valued coupling constant. This description results in a time evolution of the input state based on these constants and also reveals a non-Markovianity measure. However, no universal master equation, like its Markovian counterpart the GKSL equation, describing the non-Markovian dynamics has been found. Studying the effect of energy conservation in this collision model might be fruitful in getting answers to newly emerging questions

- Are there any effects of strict energy conservation on the system dynamics without having to solve the differential equation?
- How do the ancilla-ancilla interactions affect the found detailed balance condition?
- The Lindbladian $\mathcal{L}$ generating the semigroup map leads to Markovian dynamics. Do we need to choose a different approach such that we can avoid using the semigroup property for the derivation of a dynamic description?

Ref. [30] presents additional approaches on how to implement memory in a collision model, by introducing different types of memory effects

- ancilla-ancilla interaction
- initially correlated ancillas
- multiple collisions of one ancilla with the system

In the end, which implementation of memory in the bath best reflects reality depends on the process one wants to model. Further looking into these approaches allows for a more realistic depiction of the open system dynamics.

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A Basic Notation

Maps and operators
In general maps are denoted by calligraphic capital letters $\mathcal{A}, \mathcal{B}, \mathcal{C}, \ldots$ and operators by capital letters $A, B, C, \ldots$.

Commutators
The commutator is denoted as $[A, B] = AB - BA$
The anti-commutator is denoted as $\{A, B\} = AB + BA$

Commutators of maps
Commutation relations on the hand of maps are less common than for operators. For operators the notion of commutators can be seen as a difference of matrix multiplications in varying order when finite Hilbert space are considered. A commutation relation of maps might seem a little more abstract since maps are only defined when they act on a state or general operator of interest. In our case what we mean by writing maps in commutator brackets, is that their action commutes when acting on any arbitrary state ρ. To summarise, the following statements about arbitrary maps $\mathcal{X}$ and $\mathcal{Y}$ can be considered equivalent

$$\mathcal{X}\left[\mathcal{Y}\left[\rho\right]\right] = \mathcal{Y}\left[\mathcal{X}\left[\rho\right]\right] \;\Leftrightarrow\; \left[\mathcal{X}, \mathcal{Y}\right]\left[\rho\right] = 0 \;\Leftrightarrow\; \left[\mathcal{X}, \mathcal{Y}\right] = 0.$$

These maps could as well be seen as superoperators in a representation like the Liouville space, where states become vectors and maps are represented as operators that act on these state vectors. The commutation relation between two superoperators can then be seen as the general commutation relation in the sense that these superoperators commute in their matrix form.

Referring to subspaces
Basis elements of the environmental DOFs are refereed to by lower case Greek letters, e.g. $|\mu\rangle \equiv |\mu\rangle_E$, while basis elements of the systems DOFs are referred to as lower case Latin letters e.g. $|\ell\rangle \equiv |\ell\rangle_S$.

Summation indices
Summing over indices where one is in parenthesis, e.g. $k(\neq \ell)$ means the sum runs over all k except for the one being equal to ℓ. However, ℓ is fixed and not an additional summation index in this notation!

Omitting tensor products

For the Hamiltonians where the index already reveals the relevant subsystem it is a clear on which DOFs they act. Therefore in the products $H_{SE}H_E \equiv H_{SE}(\mathbb{1}_S \otimes H_E)$ and $H_{SE}\,\tau \equiv H_{SE}(\mathbb{1}_S \otimes \tau)$ we have omitted the tensor product sign ($\otimes$).

Natural units
We use natural units $\hbar = k_B = 1$ and therefore these constants are omitted in all equations.

B Qubit Examples

B.1 Dynamic Description of Open Quantum Systems

Starting with the following choice of Hamiltonians in $d_S = d_E = 2$

$$H_S = \sigma_z, \qquad H_E = \sigma_z \qquad H_{SE} = \sigma_+ \otimes \sigma_- + \sigma_- \otimes \sigma_+, \tag{B.1}$$

where $\sigma_+ = |0\rangle\langle 1|$ and $\sigma_- = |1\rangle\langle 0|$ and $\sigma_\pm^\dagger = \sigma_\mp$.

B.1.1 Evolution Following from the Semigroup Map

Computing the Lindblad jump operators according to Eq. (2.61) gives

$$\begin{aligned} L_{\alpha\gamma} &= \sqrt{p_\alpha}\,\langle\alpha|\,(\sigma_+ \otimes \sigma_- + \sigma_- \otimes \sigma_+)\,|\gamma\rangle \\ &= \sqrt{p_\alpha}\,(\sigma_-\delta_{0\alpha}\delta_{1\gamma} + \sigma_+\delta_{1\alpha}\delta_{0\gamma}) \end{aligned} \tag{B.2}$$

Computing the Lindbladian $\mathcal{L}$ according to Eq. (2.47) when applied to an arbitrary systems state $\rho = \sum_{i,j}\rho_{ij}\,|i\rangle\langle j|$ in parts yields

$$\begin{aligned} \sum_{\alpha,\gamma} L_{\alpha\gamma}\rho L_{\alpha\gamma}^\dagger &= \sum_{\alpha,\gamma} p_\alpha\,(\sigma_-\rho\sigma_+\delta_{0\alpha}\delta_{1\gamma} + \sigma_+\rho\sigma_-\delta_{1\alpha}\delta_{0\gamma}) \\ &= p_0\rho_{00}\,|1\rangle\langle 1| + p_1\rho_{11}\,|0\rangle\langle 0| \end{aligned} \tag{B.3}$$

All other crossterms vanish since the contain $\delta_{0\alpha}$ as well as $\delta_{1\alpha}$ which always results in zero. Similarly for the index γ. Analogous for the anti commutator part

$$\begin{aligned}
\sum_{\alpha,\gamma}\left\{L_{\alpha\gamma}^{\dagger}L_{\alpha\gamma},\rho\right\} &= \sum_{\alpha,\gamma} p_\alpha \left\{\left(\sigma_-\delta_{0\alpha}\delta_{1\gamma}+\sigma_+\delta_{1\alpha}\delta_{0\gamma}\right)\left(\sigma_-\delta_{0\alpha}\delta_{1\gamma}+\sigma_+\delta_{1\alpha}\delta_{0\gamma}\right),\rho\right\} \\
&= \sum_{\alpha,\gamma} p_\alpha \left\{\left(|1\rangle\langle 1|\,\delta_{0\alpha}\delta_{1\gamma}+|0\rangle\langle 0|\,\delta_{1\alpha}\delta_{0\gamma}\right),\rho\right\} \\
&= p_1\left(|1\rangle\langle 1|\,\rho+\rho\,|1\rangle\langle 1|\right)+p_0\left(|0\rangle\langle 0|\,\rho+\rho\,|0\rangle\langle 0|\right) \\
&= p_1\rho_{10}\,|1\rangle\langle 0|+p_1\rho_{11}\,|1\rangle\langle 1|+p_0\rho_{00}\,|0\rangle\langle 0|+p_0\rho_{01}\,|0\rangle\langle 1| \\
&\quad +p_1\rho_{01}\,|0\rangle\langle 1|+p_1\rho_{11}\,|1\rangle\langle 1|+p_0\rho_{00}\,|0\rangle\langle 0|+p_0\rho_{10}\,|1\rangle\langle 0| \\
&= 2p_0\rho_{00}\,|0\rangle\langle 0|+\rho_{01}\,|0\rangle\langle 1|+\rho_{10}\,|1\rangle\langle 0|+2p_1\rho_{11}\,|1\rangle\langle 1|\,,
\end{aligned} \tag{B.4}$$

where we used that the environment thermal state τ is of trace 1 and therefore, $p_0+p_1=1$.
The Lamb Shift Hamiltonian can be computed according to Eq. (2.70).

$$\begin{aligned}
H_{LS} &= \mathrm{tr}_E\left(\left(\sigma_+\otimes\sigma_-+\sigma_-\otimes\sigma_+\right)\tau\right) \\
&= p_0\sigma_+\mathrm{tr}\left(\sigma_-\right)+p_1\sigma_-\mathrm{tr}\left(\sigma_+\right)=0
\end{aligned} \tag{B.5}$$

since σ_+ and σ_- are both traceless. Therefore, also the Lamb shift Hamiltonian map vanishes.
The system Hamiltonian commutator can also be calculated by

$$\begin{aligned}
-i\left[H_S,\rho\right] &= -i\left(\sigma_z\rho-\rho\sigma_z\right) \\
&= -i\big(\rho_{00}\,|0\rangle\langle 0|+\rho_{01}\,|0\rangle\langle 1|-\rho_{10}\,|1\rangle\langle 0|-\rho_{11}\,|1\rangle\langle 1| \\
&\qquad -\rho_{00}\,|0\rangle\langle 0|-\rho_{10}\,|1\rangle\langle 0|+\rho_{01}\,|0\rangle\langle 1|+\rho_1\,|1\rangle\langle 1|\,\big) \\
&= 2i\left(\rho_{01}\,|0\rangle\langle 1|-\rho_{10}\,|1\rangle\langle 0|\right)
\end{aligned} \tag{B.6}$$

Plugging in Eqs. (B.3) to (B.6) into Eq. (2.47) then yields

$$\begin{aligned}
\frac{\partial\rho}{\partial t}=\mathcal{L}\left[\rho\right] =& 2i\left(\rho_{01}\,|0\rangle\langle 1|-\rho_{10}\,|1\rangle\langle 0|\right)+p_0\rho_{00}\,|1\rangle\langle 1|+p_1\rho_{11}\,|0\rangle\langle 0| \\
&-\frac{1}{2}\left(2p_0\rho_{00}\,|0\rangle\langle 0|+\rho_{01}\,|0\rangle\langle 1|+\rho_{10}\,|1\rangle\langle 0|+2p_1\rho_{11}\,|1\rangle\langle 1|\right) \\
=& \begin{pmatrix} -p_1\rho_{00}+p_0\rho_{11} & -2i\rho_{01}-\frac{1}{2}\rho_{01} \\ 2i\rho_{10}-\frac{1}{2}\rho_{10} & p_1\rho_{00}-p_0\rho_{11}\end{pmatrix}
\end{aligned} \tag{B.7}$$

To compute the action of the semi group map it is convenient to switch to the Liouville picture where the elements of a matrix are stacked on top of each

other to become vectors, while maps become matrices (superoperators).

$$|\dot{\rho}\rangle\rangle = \begin{pmatrix} -p_1\rho_{00} + p_0\rho_{11} \\ -2i\rho_{01} - \frac{1}{2}\rho_{01} \\ 2i\rho_{10} - \frac{1}{2}\rho_{10} \\ p_1\rho_{00} - p_0\rho_{11} \end{pmatrix} \tag{B.8}$$

similarly the density matrix ρ is expressed as

$$|\rho\rangle\rangle = \begin{pmatrix} \rho_{00} \\ \rho_{01} \\ \rho_{10} \\ \rho_{11} \end{pmatrix} \tag{B.9}$$

The master equation can then be rewritten to $|\dot{\rho}\rangle\rangle = \hat{L}\,|\rho\rangle\rangle$ where $\hat{L}$ is a superoperator that is a 4x4 matrix in Liouville space for this qubit example. A non-unique choice of $\hat{L}$ that solves the equation is

$$\hat{L} = \begin{pmatrix} -p_1 & 0 & 0 & p_0 \\ 0 & -2i - \frac{1}{2} & 0 & 0 \\ 0 & 0 & 2i - \frac{1}{2} & 0 \\ p_1 & 0 & 0 & -p_0 \end{pmatrix} \tag{B.10}$$

Since $\hat{L}$ is the generator of the map Λ_t we can compute it by also employing $p_0 + p_1 = 1$ and find

$$\hat{\Lambda}_t = e^{\hat{L}t} = \begin{pmatrix} 1 + (e^{-t} - 1)p_1 & 0 & 0 & (e^{-t} - 1)p_0 \\ 0 & e^{-\left(\frac{1}{2} - 2i\right)t} & 0 & 0 \\ 0 & 0 & e^{-\left(\frac{1}{2} + 2i\right)t} & 0 \\ (1 - e^{-t})p_1 & 0 & 0 & e^{-t} + (1 - e^{-t})p_1 \end{pmatrix}. \tag{B.11}$$

Which results in $\rho(t)$ by multiplying its vector in Eq. (B.9) with the matrix in Eq. (B.11)

$$|\rho(t)\rangle\rangle = \hat{\Lambda}_t\,|\rho(0)\rangle\rangle \tag{B.12}$$

We can then compute the time evolution of ρ and its expectation value w.r.t z starting in a pure ground state $\rho(0) = |0\rangle\langle 0|$

$$\langle\rho(t)\rangle_z = \mathrm{tr}\left[\rho(t)\sigma_z\right] = \left(1 - e^{-t}\right)\tanh(\beta) + e^{-t}. \tag{B.13}$$

The resulting time evolution is plotted in Figure B.1 where it is compared to the result of directly applying the dynamical map to ρ.

B.1.2 Evolution Following from the Dynamical Map

Here, we illustrate the difference in the dynamics following from the semigroup map Λ_t generated by $\hat{L}$ using Eq. (2.43) to the dynamic description of the dynamical map

$$\mathcal{E}_t[\rho] = \mathrm{tr}_E\left[U(\rho\otimes\tau)U^\dagger\right]. \tag{B.14}$$

Since τ is a positive operator the decomposition $\tau = \sqrt{\tau}\sqrt{\tau}$ is admissible. In the eigenbasis of system and environment $\{|\alpha\rangle\}$ we find that

$$\begin{aligned}\mathcal{E}_t[\rho] =& \mathrm{tr}_E\left[U(\rho\otimes\tau)U^\dagger\right]\\ =& \sum_\alpha \langle\alpha| U(\mathbb{1}_S\otimes\sqrt{\tau})(\rho\otimes\mathbb{1}_E)(\mathbb{1}_S\otimes\sqrt{\tau})U^\dagger|\alpha\rangle\\ =& \sum_{\alpha,\beta}\langle\alpha|U(\mathbb{1}_S\otimes\sqrt{\tau})|\beta\rangle\rho\langle\beta|(\mathbb{1}_S\otimes\sqrt{\tau})U^\dagger|\alpha\rangle,\end{aligned} \tag{B.15}$$

where in the third line we introduced an identity matrix. Eq. (B.15) is a Kraus decomposition of the dynamical map Λ_t. The unitary evolution can then be computed to

$$U = e^{iHt} = \begin{pmatrix} e^{-2it} & 0 & 0 & 0\\ 0 & \cos(t) & -i\sin(t) & 0\\ 0 & -i\sin(t) & \cos(t) & 0\\ 0 & 0 & 0 & e^{2it}\end{pmatrix} \tag{B.16}$$

The product with the square root of the environment thermal state then gives

$$U(\mathbb{1}_S\otimes\sqrt{\tau}) = \begin{pmatrix} e^{-2it}\sqrt{p_0} & 0 & 0 & 0\\ 0 & \sqrt{p_1}\cos(t) & -i\sqrt{p_0}\sin(t) & 0\\ 0 & -i\sqrt{p_1}\sin(t) & \sqrt{p_0}\cos(t) & 0\\ 0 & 0 & 0 & e^{2it}\sqrt{p_1}\end{pmatrix} \tag{B.17}$$

Computing the Krausoperators $K_{\mu\nu} = \langle\mu|U(\mathbb{1}_S\otimes\sqrt{\tau})|\nu\rangle$ results in

$$(K)_{\mu\nu} = \begin{pmatrix} \begin{pmatrix} e^{-2it}\sqrt{p_0} & 0\\ 0 & \sqrt{p_0}\cos(t)\end{pmatrix} & \begin{pmatrix} 0 & 0\\ -i\sqrt{p_1}\sin(t) & 0\end{pmatrix}\\ \begin{pmatrix} 0 & -i\sqrt{p_0}\sin(t)\\ 0 & 0\end{pmatrix} & \begin{pmatrix} \sqrt{p_1}\cos(t) & 0\\ 0 & e^{2it}\sqrt{p_1}\end{pmatrix}\end{pmatrix} \tag{B.18}$$

The Liouville form of the dynamical map in Kraus form is then

$$\hat{\mathcal{E}}_t = \sum_{\mu,\nu} K_{\mu\nu} \otimes K^*_{\mu\nu} = \begin{pmatrix} p_1 \cos^2(t) + p_0 & 0 & 0 & p_0 \sin^2(t) \\ 0 & \cos(t)e^{-2it} & 0 & 0 \\ 0 & 0 & \cos(t)e^{2it} & 0 \\ p_1 \sin^2(t) & 0 & 0 & p_0 \cos^2(t) + p_1 \end{pmatrix} \tag{B.19}$$

From this represenation we immediately see that the dynamics of the semi group map in Eq. (B.11) and from the dynamical map in Eq. (B.19) differ from one another. To highlight these differences we compare the dynamics form these two maps by computing the expectation value in the z direction of the state $\rho(t) = \hat{\mathcal{E}}_t \left|\rho(0)\right\rangle\rangle$ w.r.t the z-direction from an initially pure ground state $\rho(0) = |0\rangle \langle 0|$

$$\langle \rho(t) \rangle_z = \mathrm{tr}\left[\rho(t)\sigma_z\right] = \frac{1}{2}\left(1 + e^{2\beta}\cos(2t)\right)(1 - \tanh(\beta)) \tag{B.20}$$

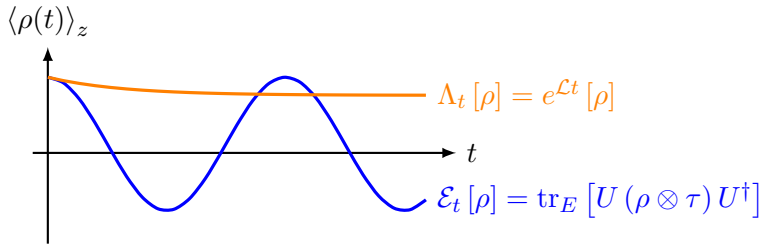

Figure B.1: Comparison of the time evolution following from a dynamical map (Eq. (B.20)) and a semigroup (Eq. (B.13)) map from an initially pure ground state $\rho(0) = |0\rangle \langle 0|$ at an inverse temperature $\beta = 1$ of the environment.

This clearly highlights the dissipative behaviour of the dynamics following from a Markovian master equation when compared to dynamics following from unitary evolution and tracing out the environment. Therefore, the dynamics of the semi group map and the dynamical map aren't necessarily equivalent.

B.2 Detailed Balance in an Energy Conserving Open Quantum System Following from a Microscopic Description

In a setup where

$$H_S = \sigma_z, \quad H_E = \sigma_z, \quad H_{SE} = \sigma_+ \otimes \sigma_- + \sigma_- \otimes \sigma_+ \tag{B.21}$$

we know that it fulfils SEC as in Eq. (2.72). By employing $\sigma_\pm = \sigma_x \pm i\sigma_y$ we can rewrite the interaction Hamiltonian

$$H_{SE} = \frac{1}{2}(\sigma_x \otimes \sigma_x + \sigma_y \otimes \sigma_y) = \sum_\alpha A_\alpha \otimes B_\alpha \tag{B.22}$$

where $A_\alpha = A_\alpha^\dagger$ and $B_\alpha = B_\alpha^\dagger$. From this most general form of the interaction Hamiltonian we can read off that

$$(B_\alpha) = \frac{1}{\sqrt{2}}(\sigma_x, \sigma_y)\,. \tag{B.23}$$

Plugging in these terms into the kinetic coefficients in Eq. (3.139) of Ref. [7] the Fourier transformation then reads on hand of the example of $\alpha = 0$ and $\beta = 1$

$$\gamma_{01}(\omega) = \int_{-\infty}^{\infty} ds\; e^{i\omega s} \frac{i\left(-e^{\beta\omega_0} e^{-i\omega_0 s} + e^{i\omega_0 s}\right)}{2\left(e^{\beta\omega_0}+1\right)} \tag{B.24}$$

and use the Fourier transform $\mathcal{F}\left[e^{i\omega_0 t}\right] = \pi\delta(\omega - \omega_0)$, where $\delta(\omega-\omega_0)$ is the Dirac delta function that is only non-vanishing for $\omega = \omega_0$. By computing the ratio of the kinetic coefficients we find

$$\frac{\gamma_{\alpha\beta}(\omega)}{\gamma_{\beta\alpha}(-\omega)} = \frac{i\sqrt{\frac{\pi}{2}}\delta(\omega+\omega_0) - i\sqrt{\frac{\pi}{2}}e^{\beta\omega_0}\delta(\omega-\omega_0)}{i\sqrt{\frac{\pi}{2}}e^{\beta\omega_0}\delta(\omega+\omega_0) - i\sqrt{\frac{\pi}{2}}\delta(\omega-\omega_0)} \tag{B.25}$$

When plugging in $\omega = \omega_0 = \varepsilon' - \varepsilon = 2$, where ε are the eigenenergies of the systems Hamiltonian in Eq. (B.21) we find that

$$\frac{\gamma_{\alpha\beta}(\omega_0)}{\gamma_{\beta\alpha}(-\omega_0)} = \frac{-i\sqrt{\frac{\pi}{2}}e^{\beta\omega_0}\delta(\omega_0-\omega_0)}{-i\sqrt{\frac{\pi}{2}}\delta(\omega_0-\omega_0)} = e^{\beta\omega_0} \tag{B.26}$$

Similarly for $\omega = -\omega_0$ we find that

$$\frac{\gamma_{\alpha\beta}(-\omega_0)}{\gamma_{\beta\alpha}(\omega_0)} = \frac{i\sqrt{\frac{\pi}{2}}\delta(-\omega_0+\omega_0)}{i\sqrt{\frac{\pi}{2}}e^{\beta\omega_0}\delta(-\omega_0+\omega_0)} = e^{-\beta\omega_0}. \tag{B.27}$$

These two equation then immediately show that detailed balance also holds for the strict energy conserving set of Hamiltonians in Eq. (B.21).
However if we chose a setup where $H_E = 2\sigma_z$, the energy gaps in the environment are $\omega_0 = \pm 4$. However, there is no energy gap in the system's energylevels for $H_S = \sigma_z$ matching the environment's and Eq. (B.25) doesn't result in a detailed balance condition. Therefore, with this interaction Hamiltonian H_{SE} non-matching energy gaps in the system and environment free Hamiltonians mean that detailed balance doesn't hold.

C Sidenotes to Calculations

C.1 Interpretation of Strict Energy Conservation

To try to implement strict energy conservation lets consider the commutation relation it in its spectral form

$$\begin{aligned}[H_{SE}, H_S + H_E] = \\ &= \left[\sum_{k,\mu,\ell,\nu} c_{k\mu\ell\nu} \left|k\right\rangle \left\langle \ell\right| \otimes \left|\mu\right\rangle \left\langle \nu\right|, \sum_i \varepsilon_i \left|i\right\rangle \left\langle i\right| + \sum_\gamma \epsilon_\gamma \left|\gamma\right\rangle \left\langle \gamma\right| \right] \\ &= \sum_{k,\mu,\ell,\nu} c_{k\mu\ell\nu} \left|k\right\rangle \left\langle \ell\right| \otimes \left|\mu\right\rangle \left\langle \nu\right| (\varepsilon_\ell - \varepsilon_k + \epsilon_\nu - \epsilon_\mu) = 0.\end{aligned} \tag{C.1}$$

By computing the expectation value for individual basis elements of system and environment we find that

$$\begin{aligned}\left\langle i\right| \left\langle \alpha\right| [H_{SE}, H_S + H_E] \left|j\right\rangle \left|\gamma\right\rangle = \\ c_{ij\alpha\gamma} (\varepsilon_j - \varepsilon_i + \epsilon_\gamma - \epsilon_\alpha) = 0,\end{aligned} \tag{C.2}$$

which simply states that an energy change in the environment has to be met in the system

$$\varepsilon_j - \varepsilon_i = -\epsilon_\gamma + \epsilon_\alpha. \tag{C.3}$$

This result shows that any energy change in the system has to be met by an equal energy change in the environment and by that no energy is lost at the interface between system and environment.

C.2 Properties of a Hermitian Matrix (α_{ij})

For arbitrary two-dimensional diagonal system and environment Hamiltonians and an interaction Hamiltonian

$$H_{SE} = \begin{pmatrix} 1 & 1+i & 0 & 0 \\ 1-i & 3 & 0 & 0 \\ 0 & 0 & 5 & 2+i \\ 0 & 0 & 2-i & 6 \end{pmatrix}, \tag{C.4}$$

with the help of Eq. (3.51) we find a Hermitian matrix α by

$$(\alpha_{kl}) = \begin{pmatrix} 3p_0 + 11p_1 & (8-i)p_0 + (21+i)p_1 \\ (8+i)p_0 + (21-i)p_1 & 30p_0 + 41p_1 \end{pmatrix} = (\alpha_{kl})^\dagger. \tag{C.5}$$

Here we want to mention that only block diagonal elements contribute to α, since only matrix elements $c_{k\nu k\mu}$ of the interaction Hamiltonian H_{SE} contribute to the resulting matrix α_{kl}.
On the other hand we know that if H_{SE} is real symmetric, α is also real symmetric. The other way around is not always true as proven by the following counter-example with arbitrary two-dimensional system and environment Hamiltonians and an interaction Hamiltonian

$$H_{SE} = \begin{pmatrix} 0 & -i & 0 & -i \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & -i \\ i & 0 & i & 0 \end{pmatrix}. \tag{C.6}$$

Applying equation (3.51) to the chosen set of Hamiltonians leads to

$$(\alpha_{k\ell}) = \begin{pmatrix} p_0 + p_1 & p_0 + p_1 \\ p_0 + p_1 & p_0 + p_1 \end{pmatrix}. \tag{C.7}$$

This is a real symmetric matrix despite a chosen non-real Hermitian H_{SE}.

D Code

D.1 Mathematica Notebook for Construction of DB-Compliant Hamiltonians

This Mathematica Notebook can be used to construct Hamiltonians from a DB compliant ME and then checks if they also fulfil SEC.

Derive Detailed Balance Compliant Sets of Hamiltonians

```
In[•]:= dS = 2;
        dE = dS;
        energiesSys = Table[ε_i, {i, 1, dS - 1}];
        energiesEnv = Table[ϵ_i, {i, 1, dS - 1}];
        HSvec = Append[{0}, energiesSys] // Flatten;
        HEvec = Append[{0}, energiesEnv] // Flatten;
        kls = Flatten[Table[If[k ≥ l, ## &[], {k, l}], {k, 0, dS - 1}, {l, 0, dS - 1}], 1]
Out[•]=
        {{0, 1}}
```

---

computing all possible combinations of ν and μ and then finding the solvable ones.

```
In[•]:= numus = Flatten[Table[Tuples[Map[Permutations, pair]], {pair, Permutations[kls]}], 1];
        Dimensions[numus];
        numus
Out[•]=
        {{{0, 1}}, {{1, 0}}}

In[•]:= eqns = Table[HSvec[[kls[[j, 1]] + 1]] - HSvec[[kls[[j, 2]] + 1]] ==
            HEvec[[numus[[i, j, 1]] + 1]] - HEvec[[numus[[i, j, 2]] + 1]], {i, 1, Length[numus]}, {j, 1, Length[kls]}];

In[•]:= sols = Table[Solve[eqns[[i]], energiesEnv], {i, 1, Length[eqns]}];
        Flatten[sols, 1]
Out[•]=
        {{ϵ_1 → ε_1}, {ϵ_1 → -ε_1}}

In[•]:= solvable = Table[If[sols[[i]] == {}, 0, 1], {i, 1, Length[eqns]}];
        solvablePos = Position[solvable, 1] // Flatten
        Length[solvablePos];
Out[•]=
        {1, 2}

In[•]:= newHEvecs = Table[If[sols[[j]] == {}, 0,
            Append[{0}, Table[Replace[ϵ_i, sols[[j, 1]]], {i, 1, dE - 1}]] // Flatten], {j, 1, Length[eqns]}];
        newHEvecs[[solvablePos]];
```

---

comparing the DB compatible solutions to the equations with the resulting HE

```
In[•]:= Print["diagonals of HE: ", newHEvecs[[solvablePos]] // MatrixForm, ", unsolved equations: ",
          eqns[[solvablePos]] // TraditionalForm, ", sets of {ν,μ}: ", numus[[solvablePos]] // TraditionalForm]
        numus[[solvablePos]];
```

diagonals of HE: $\begin{pmatrix} 0 & \varepsilon_1 \\ 0 & -\varepsilon_1 \end{pmatrix}$, unsolved equations: $\begin{pmatrix} -\varepsilon_1 = -\epsilon_1 \\ -\varepsilon_1 = \epsilon_1 \end{pmatrix}$, sets of $\{\nu,\mu\}$: $\begin{pmatrix} \{0, 1\} \\ \{1, 0\} \end{pmatrix}$

computing HSE and checking if the DB compliant set of Hamiltonians fulfils strict energy

```
In[•]:= PartialTrace[matrix_, d_, sys_] := Module[{partialTr, i, j, k}, partialTr = ConstantArray[0, {d, d}];
  Which[sys == 2 (*Trace over the second subsystem*), For[i = 1, i ≤ d, i++, For[j = 1, j ≤ d, j++,
      For[k = 1, k ≤ d, k++, partialTr[[i, j]] += matrix[[d * (i - 1) + k, d * (j - 1) + k]];];];],
   sys == 1(*Trace over the first subsystem*), For[i = 1, i ≤ d, i++, For[j = 1, j ≤ d, j++,
      For[k = 1, k ≤ d, k++, partialTr[[i, j]] += matrix[[d * (k - 1) + i, d * (k - 1) + j]];];];]];
  partialTr]
```

```
In[•]:= SECiffDB = {};
HSEs = {};
LambShiftZero = {};
For[j = 1, j ≤ Length[solvablePos], j++,
 HSE = ArrayFlatten[Table[If[Or @@ Table[And[l == kls[[i, 2]], ν == numus[[solvablePos[[j]], i, 1]],
        k == kls[[i, 1]], μ == numus[[solvablePos[[j]], i, 2]]], {i, dE * (dE - 1) / 2}],
     Subscript[c, k, μ, l, ν], 0], {k, 0, dS - 1}, {l, 0, dS - 1}, {μ, 0, dE - 1}, {ν, 0, dE - 1}]];
 HSE = HSE + ConjugateTranspose[HSE];
 HE = DiagonalMatrix[newHEvecs[[solvablePos[[j]]]]];
 Tau = MatrixExp[(-β) * HE];
 identTau = IdentityMatrix[dS] ⊗ Tau / Tr[Tau] // ArrayFlatten;
 trVt = PartialTrace[HSE.identTau, dS, 2](*Trace over 1==System, 2==Environment*);
 HSpHE = ArrayFlatten[TensorProduct[DiagonalMatrix[HSvec], IdentityMatrix[dE]] +
    TensorProduct[IdentityMatrix[dS], DiagonalMatrix[newHEvecs[[solvablePos[[j]]]]]]];
 Print["HS=", DiagonalMatrix[HSvec] // TraditionalForm, " , HE=",
  DiagonalMatrix[newHEvecs[[solvablePos[[j]]]] // TraditionalForm, " , V=", HSE // TraditionalForm,
  ", Tr_E(Vτ)= ", trVt // TraditionalForm, " follow from detailed balance and",
  If[HSpHE.HSE == HSE.HSpHE, Style[" fulfil", Underlined, Bold], " don't fulfil"],
  " strict energy conservation. "];
 AppendTo[SECiffDB, If[HSpHE.HSE == HSE.HSpHE, "yes", "no"]];
 AppendTo[LambShiftZero, If[trVt == ConstantArray[0, {dS, dS}], "yes", "no"]];
 AppendTo[HSEs, HSE];
]
```

$$HS=\begin{pmatrix}0 & 0\\ 0 & \varepsilon_1\end{pmatrix},\ HE=\begin{pmatrix}0 & 0\\ 0 & \varepsilon_1\end{pmatrix},\ V=\begin{pmatrix}0 & 0 & 0 & 0\\ 0 & 0 & c_{0,1,1,0} & 0\\ 0 & (c_{0,1,1,0})^* & 0 & 0\\ 0 & 0 & 0 & 0\end{pmatrix},\ \mathrm{Tr}_E(V\tau)=$$

$\begin{pmatrix}0 & 0\\ 0 & 0\end{pmatrix}$ follow from detailed balance and **fulfil** strict energy conservation.

$$HS=\begin{pmatrix}0 & 0\\ 0 & \varepsilon_1\end{pmatrix},\ HE=\begin{pmatrix}0 & 0\\ 0 & -\varepsilon_1\end{pmatrix},\ V=\begin{pmatrix}0 & 0 & 0 & c_{0,0,1,1}\\ 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\\ (c_{0,0,1,1})^* & 0 & 0 & 0\end{pmatrix},\ \mathrm{Tr}_E(V\tau)=$$

$\begin{pmatrix}0 & 0\\ 0 & 0\end{pmatrix}$ follow from detailed balance and **fulfil** strict energy conservation.

E Derivations

E.1 Calculations for Coefficient Contribution Analysis

We will start this analysis with the results from the unitary invariant spectrum. Here, we will find a condition that allows us to eliminate some coefficients right away. Therefore, we will first consider the case $k = \ell$ where we found the condition relating $a_{nmn'm'}$ to $b_k^{k'}$ in Eq. (3.43) and discuss its implications first. Afterwards we will do the same for the case $k \neq \ell$ where the $a_{nmn'm'}$ are related to f_{nm} in Eq. (3.41). We will perform this analysis systematically and consider every relevant combination of index pairs being equivalent or not. So, starting with the first case $k = \ell$ and Eq. (3.43) we can distinguish the following subcases.

- $k' \neq \ell'$: This restriction reduces Eq. (3.43) to

$$a_{k'kk\ell'} - \frac{1}{2}\sum_m \left(a_{k'mmk}\delta_{k\ell'} + a_{kmm\ell'}\delta_{kk'}\right) = 0 \tag{E.1}$$

  - $k \neq k'$ and $k \neq \ell'$:

$$a_{k'kk\ell'} = 0 \tag{E.2}$$

  - $k = \ell' \Rightarrow k \neq k'$:

$$a_{k'\ell'\ell'\ell'} - \frac{1}{2}\sum_m a_{k'mm\ell'} = 0 \tag{E.3}$$

  - $k = k' \Rightarrow k \neq \ell'$

$$a_{k'k'k'\ell'} - \frac{1}{2}\sum_m a_{k'mm\ell'} = 0 \tag{E.4}$$

- $k' = \ell'$: This restriction reduces Eq. (3.43) to

$$a_{k'kkk'} - \frac{1}{2}\sum_m \left(a_{k'mmk}\delta_{kk'} + a_{kmmk'}\delta_{kk_0}\right) = b_{k'}^{(k)} \tag{E.5}$$

- $k = k'$

$$\begin{aligned} a_{kkkk} - \frac{1}{2}\sum_m (a_{kmmk} + a_{kmmk}) &= b_k^{(k)} \\ a_{kkkk} - \left(a_{kkkk} + \sum_{m(\neq k)} a_{kmmk} \right) &= b_k^{(k)} \\ - \sum_{m(\neq k)} a_{kmmk} &= b_k^{(k)} \end{aligned} \tag{E.6}$$

- $k \neq k'$

$$a_{k'kkk'} = b_{k'}^{(k)} \tag{E.7}$$

Here Eqs. (E.3) and (E.4) both lead to the same result when the indices are matched and by that both lead to

$$a_{k'\ell'\ell'\ell'} = a_{k'k'k'\ell'}. \tag{E.8}$$

This can be seen on hand of Eq. (E.3) by extracting the two terms where $m = k'$ and $m = \ell'$ out of the sum over m.

$$a_{k'\ell'\ell'\ell'} - \frac{1}{2}\left(a_{k'\ell'\ell'\ell'} + a_{k'k'k'\ell'} + \sum_{m(\neq k',\ell')} \cancelto{0}{a_{k'mm\ell'}} \right) = 0 \tag{E.9}$$

Here we used Eq. (E.2) to eliminate all the remaining terms in the sum. This and a similar calculation starting from Eq. (E.4) immediately result in Eq. (E.8).

To summarize, the case study for $k = \ell$, Eqs. (E.6) to (E.8) tell us that the coefficients with index combinations $a_{k\ell\ell k}$, $a_{kkk\ell}$ and $a_{k\ell\ell\ell}$ can be non-zero in general and still fulfill the conditions in Eqs. (3.25) and (3.26), that are a direct consequence of the thermodynamic setup of the CM.

For the case $k \neq \ell$ that leads to the condition in (3.41) a study of the following subcases suffices.

- $k = k'$ and $\ell \neq \ell_0$

$$a_{kk\ell\ell'} - \frac{1}{2}\sum_m a_{\ell mm\ell'} = 0 \tag{E.10}$$

- $k \neq k'$ and $\ell = \ell'$

$$a_{k'k\ell\ell} - \frac{1}{2}\sum_m a_{k'mmk} = 0 \tag{E.11}$$

- $k \neq k'$ and $\ell \neq \ell'$

$$a_{k'k\ell\ell'} = 0 \tag{E.12}$$

- $k = k'$ and $\ell = \ell'$

$$a_{kk\ell\ell} - \frac{1}{2}\sum_m \left(a_{kmmk} + a_{\ell mm\ell}\right) = f_{k\ell} \tag{E.13}$$

From Eq. (E.10) we find that

$$a_{kk\ell\ell'} - \frac{1}{2}\left(a_{\ell\ell'\ell'\ell'} + a_{\ell\ell\ell\ell'} + \sum_{m(\neq\ell,\ell')} \cancelto{0}{a_{\ell mm\ell'}}\right) = 0 \tag{E.14}$$

This result was found by extracting the terms where $m = \ell$ and $m = \ell'$ out of the sum and employing Eq. (E.2) to see that the remaining elements are all zero individually.
Applying this conclusion to the results of Eq. (E.8) implies that

$$a_{kk\ell\ell'} = a_{\ell\ell\ell\ell'} = a_{\ell\ell'\ell'\ell'} \;\forall\; k \neq \ell, \ell \neq \ell'. \tag{E.15}$$

A similar calculation as in Eq. (E.14) can be done on the basis of Eq. (E.11) which leads to

$$a_{k'k\ell\ell} - \frac{1}{2}\left(a_{k'k'k'k} + a_{k'kkk} + \sum_{m(\neq k,k')} \cancelto{0}{a_{k'mmk}}\right) = 0. \tag{E.16}$$

By again employing Eq. (E.8) we find that

$$a_{k'k\ell\ell} = a_{k'k'k'k} = a_{k'kkk} \;\forall\; k' \neq k,\; k \neq \ell. \tag{E.17}$$

When matching the indices of Eqns. (E.15) and (E.17) they can be brought together and reveal a final restriction following from SEC on the four-index coefficients $a_{nmn'm'}$ that can be written as

$$a_{kkk\ell} = a_{k\ell\ell\ell} = a_{k\ell nn} = a_{mmk\ell} \;\forall\; k \neq \ell,\; \ell \neq n,\; k \neq m. \tag{E.18}$$

E.2 Terms Contributing to the Overall Dynamics

Since we want to show that all the terms beside $a_{k\ell\ell k}$ and $a_{kk\ell\ell}$ vanish in the dissipator we will start by considering the third line of Eq. (3.45) acting on elements of the non-invariant basis (transition operators F_{nm}).

E.2.1 Dissipator $\mathcal{D}$ Acting on Transition Operators

- third line

$$\begin{aligned}\sum_{k\neq\ell} a_{kkk\ell}\left(|k\rangle\langle k|i\rangle\langle j|k\rangle\langle\ell| - \frac{1}{2}\left\{|k\rangle\langle k|k\rangle\langle\ell|, |i\rangle\langle j|\right\}\right)\\ = -\frac{1}{2}\left(\sum_k a_{kkki}|k\rangle\langle j| + \sum_\ell a_{jjj\ell}|i\rangle\langle\ell|\right)\end{aligned} \tag{E.19}$$

- fourth line

$$\begin{aligned}\sum_{k\neq\ell} a_{k\ell\ell\ell}\left(|k\rangle\langle\ell|i\rangle\langle j|\ell\rangle\langle\ell| - \frac{1}{2}\left\{|k\rangle\langle\ell|\ell\rangle\langle\ell|, |i\rangle\langle j|\right\}\right)\\ = -\frac{1}{2}\left(\sum_k a_{kiii}|k\rangle\langle j| + \sum_\ell a_{j\ell\ell\ell}|i\rangle\langle\ell|\right)\end{aligned} \tag{E.20}$$

- fifth line

$$\begin{aligned}\sum_{k\neq\ell,\ell\neq m} a_{k\ell mm}\left(|k\rangle\langle\ell|i\rangle\langle j|m\rangle\langle m| - \frac{1}{2}\left\{|k\rangle\langle\ell|m\rangle\langle m|, |i\rangle\langle j|\right\}\right)\\ = \sum_k a_{kijj}|k\rangle\langle j|\end{aligned} \tag{E.21}$$

- sixth line

$$\begin{aligned}\sum_{k\neq\ell,\ell\neq m} a_{kk\ell m}\left(|k\rangle\langle k|i\rangle\langle j|\ell\rangle\langle m| - \frac{1}{2}\left\{|k\rangle\langle k|\ell\rangle\langle m|, |i\rangle\langle j|\right\}\right)\\ = \sum_m a_{iijm}|i\rangle\langle m|\end{aligned} \tag{E.22}$$

Lines three to six of Eq. (3.45) when acting on transition operators can be combined to

$$
\begin{aligned}
&-\frac{1}{2}\left(\sum_{k(\neq i)} a_{kkki}\,|k\rangle\langle j| + \sum_{k(\neq j)} a_{jjjk}\,|i\rangle\langle k|\right) - \frac{1}{2}\left(\sum_{k(\neq i)} a_{kiii}\,|k\rangle\langle j| + \sum_{k(\neq j)} a_{jkkk}\,|i\rangle\langle k|\right) \\
&\qquad + \sum_{k(\neq i)} a_{kijj}\,|k\rangle\langle j| + \sum_{k(\neq j)} a_{iijk}\,|i\rangle\langle k| \\
=&\frac{1}{2}\left(\sum_{k(\neq i)} \left(2a_{kijj} - a_{kkki} - a_{kiii}\right)|k\rangle\langle j| + \sum_{k(\neq j)} \left(2a_{iijk} - a_{jjjk} - a_{jkkk}\right)|i\rangle\langle k|\right) = 0.
\end{aligned}
\tag{E.23}
$$

Combining these lines yields zero since Eq. (3.44) implies that both terms in the last line of Eq. (E.23) are zero individually.
Since equation (E.23) only holds for $i \neq j$ a similar consideration needs to be performed when considering Eq. (3.45) acting on elements from the invariant part of the basis (projection operators Π_i).

E.2.2 Disspator $\mathcal{D}$ Acting on Projection Operators

- third line

$$
\begin{aligned}
&\sum_{k\neq\ell} a_{kkk\ell}\left(|k\rangle\langle k|i\rangle\langle i|k\rangle\langle\ell| - \frac{1}{2}\left\{|k\rangle\langle k|k\rangle\langle\ell|, |i\rangle\langle i|\right\}\right) \\
&\qquad = \sum_{\ell} a_{iii\ell}\,|i\rangle\langle\ell| - \frac{1}{2}\left(\sum_{k} a_{kkki}\,|k\rangle\langle i| + \sum_{\ell} a_{iii\ell}\,|i\rangle\langle\ell|\right).
\end{aligned}
\tag{E.24}
$$

- fourth line

$$
\begin{aligned}
&\sum_{k\neq\ell} a_{k\ell\ell\ell}\left(|k\rangle\langle\ell|i\rangle\langle i|\ell\rangle\langle\ell| - \frac{1}{2}\left\{|k\rangle\langle\ell|\ell\rangle\langle\ell|, |i\rangle\langle i|\right\}\right) \\
&= \sum_{k} a_{kiii}\,|k\rangle\langle i| - \frac{1}{2}\left(\sum_{k} a_{kiii}\,|k\rangle\langle i| + \sum_{\ell} a_{i\ell\ell\ell}\,|i\rangle\langle\ell|\right)
\end{aligned}
\tag{E.25}
$$

- fifth line

$$
\sum_{k\neq\ell,\ell\neq m} a_{k\ell mm}\left(|k\rangle\langle\ell|i\rangle\langle i|m\rangle\langle m| - \frac{1}{2}\left\{|k\rangle\langle\ell|m\rangle\langle m|, |i\rangle\langle i|\right\}\right) = 0
\tag{E.26}
$$

- sixth line

$$\sum_{k\neq\ell,\ell\neq m} a_{kk\ell m}\left(|k\rangle\langle k|i\rangle\langle i|\ell\rangle\langle m| - \frac{1}{2}\left\{|k\rangle\langle k|\ell\rangle\langle m|, |i\rangle\langle i|\right\}\right) = 0 \quad \text{(E.27)}$$

Similar as for the transition operators, when lines three to six of equation (3.45) are combined they equate to

$$\begin{aligned}
&\sum_{\ell(\neq i)} a_{iii\ell}\,|i\rangle\langle\ell| - \frac{1}{2}\left(\sum_{k(\neq i)} a_{kkki}\,|k\rangle\langle i| + \sum_{\ell(\neq i)} a_{iii\ell}\,|i\rangle\langle\ell|\right) \\
&\qquad + \sum_{k(\neq i)} a_{kiii}\,|k\rangle\langle i| - \frac{1}{2}\left(\sum_{k(\neq i)} a_{kiii}\,|k\rangle\langle i| + \sum_{\ell(\neq i)} a_{i\ell\ell\ell}\,|i\rangle\langle\ell|\right) \qquad \text{(E.28)} \\
&= \frac{1}{2}\sum_{k(\neq i)} (a_{kiii} - a_{kkki})\,|k\rangle\langle i| + \frac{1}{2}\sum_{\ell(\neq i)} (a_{iii\ell} - a_{i\ell\ell\ell})\,|i\rangle\langle\ell| = 0.
\end{aligned}$$

Combining lines three to six of Eq. (3.45) again yields zero since by Eq. (E.18) both terms in the last line of Eq. (E.28) are zero individually.

E.2.3 Consequences of a Real Matrix $(\alpha_{k\ell})$

Studying the special case of α being a real symmetric matrix allows for a further simplification of $\mathcal{D}_\Pi$ in Eq. (3.48). This simplification can be achievied by diagonalizing α via a similarity transformation $Q\alpha Q^T = \mathrm{diag}\,(\lambda_1, \ldots, \lambda_{d_S})$ where Q are orthogonal matrices. Since orthogonal matrices are real, any operator of the form

$$M_j = \sum_i Q_{ij}\Pi_i \qquad \text{(E.29)}$$

is a Hermitian matrix with real eigenvalues. Substituting $\alpha_{k\ell}$ in the $\mathcal{D}_\Pi$ part of Eq. (3.48) with its similarity transformation yields

$$
\begin{aligned}
&\sum_{\ell,k} \alpha_{k\ell} \left(\Pi_k \bullet \Pi_\ell - \frac{1}{2} \{\Pi_k \Pi_\ell, \bullet\} \right) = \\
&\quad = \sum_j \sum_{\ell,k} Q_{kj} \lambda_j \left(Q_{j\ell}\right)^T \left(\Pi_k \bullet \Pi_\ell - \frac{1}{2} \{\Pi_k \Pi_\ell, \bullet\} \right) \\
&\quad = \sum_j \lambda_j \left(\sum_k Q_{kj} \Pi_k \bullet \sum_\ell Q_{\ell j} \Pi_\ell - \frac{1}{2} \left\{ \sum_k Q_{kj} \Pi_k \sum_\ell Q_{\ell j} \Pi_\ell, \bullet \right\} \right) \\
&\quad = -\frac{1}{2} \sum_j \lambda_j \left(-M_j \bullet M_j + M_j M_j \bullet + \bullet M_j M_j - M_j \bullet M_j \right) \\
&\quad = -\frac{1}{2} \sum_j \lambda_j \left[M_j, M_j \bullet - \bullet M_j \right] \\
&\quad = -\frac{1}{2} \sum_j \lambda_j \left[M_j, \left[M_j, \bullet \right] \right].
\end{aligned}
\tag{E.30}
$$

Here we substituted each product of orthogonal matrix Q and projection operator Π_i with the Hermitian operator M_j as defined in Eq. (E.29). Expressing the dephasing part of the dissipator in Eq. (3.47) as in Eq. (E.30) therefore allows for a further simplification by collapsing the sum over two indices to just one index.

The matrix α can experience complex values as well, as can be seen in Section 3.5.6. Diagonalizing Hermitian matrices α that are not real symmetric by a similarity transformation does not allow for the same simplification as in Eq. (E.30). General Hermitian matrices can be diagonalized by a unitary similarity transformation $U \alpha U^\dagger = \mathrm{diag}\left(\lambda_1, \ldots, \lambda_{d_S}\right)$, where the matrices U are unitary. This implies that any operator of the form $V_n = \sum_i U_{in} \Pi_i$ is a matrix that can experience complex eigenvalues. Substituting $\alpha_{k\ell}$ in the dephasing part of Eq. (3.48) with the unitary similarity transformation leads to problems when trying to further simplify the equation

$$\begin{aligned}
\sum_{\ell,k} \alpha_{k\ell} \left(\Pi_k \bullet \Pi_\ell - \frac{1}{2} \{\Pi_k \Pi_\ell, \bullet\} \right) = \\
&= \sum_j \sum_{\ell,k} U_{kj} \lambda_j \left(U^*_{j\ell}\right)^T \left(\Pi_k \bullet \Pi_\ell - \frac{1}{2} \{\Pi_k \Pi_\ell, \bullet\} \right) \\
&= \sum_j \lambda_j \left(\sum_k U_{kj} \Pi_k \bullet \sum_\ell U^*_{\ell j} \Pi_\ell - \frac{1}{2} \left\{ \sum_k U_{kj} \Pi_k \sum_\ell U^*_{\ell j} \Pi_\ell, \bullet \right\} \right) \\
&= -\frac{1}{2} \sum_j \lambda_j \left(-V_j \bullet V_j^* + V_j V_j^* \bullet + \bullet V_j V_j^* - V_j \bullet V_j^* \right).
\end{aligned} \tag{E.31}$$

It can now be seen that, if α is not a real symmetric matrix it is not possible to simplify the dissipator in a meaningful manner.

We want to stress again that Eq. (E.30) only holds for real symmetric α and no further simplification of the dissipator is possible for general Hermitian α. The matrix α is certainly not always real valued, but one case where $\alpha_{k\ell}$ are real is for real symmetric H_{SE} in the eigenbasis of $H_S + H_E$.