

QUANTUM MARKOV SEMIGROUPS AND THE LINDBLAD MASTER EQUATION

A GENERALISATION TO COUNTABLY INFINITE DIMENSIONAL HILBERT SPACES
OF THE LINDBLAD FORM FOR GENERATORS COMMUTING WITH THE MODULAR
AUTOMORPHISM GROUP

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To infinity and beyond!

B. Lightyear

ABSTRACT

Quantum Markov Semigroups (QMS) describe the evolution of a quantum system by evolving a projection or density operator in time. QMS are generated by a generator obeying the well-known Lindblad equation. However, this is a difficult equation. Therefore, the result that the Lindblad form greatly simplifies in the case of the generator commuting with the modular automorphisms group, is useful. Unfortunately, the proof only works for finite dimensional Hilbert spaces, which is why the aim of this thesis is to generalise this result to countably infinite dimensional Hilbert spaces. To this end, the Lindblad equation is derived from both a mathematical and physical perspective. Where the former relies on rigorous proof and the latter relies on approximations.

In the rigorous case the theory of unital completely positive maps is used. Furthermore, multiple topologies are considered which put less stringent conditions on the operators of interest than the norm topology. Additionally, the Haar measure is used on the unitaries of the bounded linear operators to construct the explicit Lindblad form.

To derive the result by employing physical assumptions the interaction picture is used. The physical derivation starts from the Von Neumann equation and uses multiple assumptions to obtain the final Lindblad form. The most important physical assumptions are: the Born approximation, the Markov approximation and the rotating wave approximation.

Furthermore, the main result is the generalisation of the simplified Lindblad form. This simplified form holds for generators commuting with the modular automorphisms group in case the Hilbert spaces are countably infinite dimensional. However, this requires the domain of the generator to be restricted to trace class operators with the identity operator artificially added. Additionally, the generator needs to map strongly convergent sequences to weakly convergent sequences. It also needs to be self-adjoint with respect to the Hilbert-Schmidt inner product. Lastly, the generator is assumed to be self-adjoint with respect to the Gelfand-Naimark-Segal (GNS) inner product $\langle X, Y \rangle = \text{Tr}(\sigma X^* Y)$ for σ a density operator. This last assumption implies that the generator commutes with the modular automorphisms group, which is the symmetry we are considering. Hence, the two previous assumptions are the additional requirements needed to generalise the result, besides the restriction of the domain. Therefore, it is recommended for further research to generalise the result for the domain extended to the bounded operators $B(\mathcal{H})$. It should be noted that the proof heavily relies on the Hilbert space structure induced by the Hilbert-Schmidt inner product. Consequently, the generalisation for the bounded operators would probably require a different approach. Another recommendation is to try and lift the sequence and self-adjoint requirements on the generator. In addition, it is interesting to investigate which physical systems actually have the symmetry of generators commuting with the modular automorphisms group.

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INTRODUCTION

In the first half of the 20th century renowned mathematician and physicist John von Neumann developed the theory of operator algebras as a mathematical foundation to understand the theory of quantum mechanics: the theory of the smallest particles and length scales, which exhibits many counter-intuitive phenomena. For instance the way a particle exhibits both particle-like and a wave-like properties, depending on which way it is measured. Quantum physics theory was first developed by some of the most famous people in physics, Paul Dirac, Erwin Schrödinger, Niels Bohr and so many others. Von Neumann expanded the theory and since his the time many physicists and mathematicians have advanced the field of quantum mechanics and it has found widespread applications in electronics, imaging and communications. However, there are still open questions and one of the interesting directions still being researched is the theory of open quantum systems. This theory describes systems that not only have an internal time evolution, but can also interact in some way with an environment. Usually, the environment is taken to be a heat bath, with which the system of interest can interact by absorbing or emitting energy.

To describe such systems, usually the density matrix formalism is used. The density matrix contains all probabilities and information regarding the statistical distribution of states within a given system. For a closed system, the density matrix evolves in time according to the Von Neumann equation, which is dependent on the Hamiltonian of the system. However, for an open quantum system the density matrix evolves along an operator called the Lindbladian, which incorporates both internal evolution and external influences. This Lindbladian generates a Quantum Markov Semigroup, which is the solution to the differential equation $d\rho/dt = L\rho$, where L is the Lindbladian and ρ a density operator. Hence, we call the Lindbladian a generator. One of the major advances in the theory of open quantum systems came in 1975, when both Lindblad [16] and Gorini, Kossakowski and Sudarshan [11] derived the equation describing the generators of the Quantum Markov Semigroups of open quantum systems. However, this equation is rather difficult. Hence, immediately after the paper was released physicists, as they often do, tried to exploit symmetries to better understand and possibly simplify the Lindblad form, which is the equation describing the generator. In 1976 Alicki [1] managed to make use of the commutation with the modular automorphisms group, which describes time evolution of an operator or density matrix in quantum mechanics, to greatly simplify the Lindblad form. His proof was generalised by Carlen and Maas in 2017 [6], but this form was only valid for finite dimensional Hilbert spaces. Hence, the main aim of this paper is to first derive the Lindblad equation from basic principles from both the mathematical and physical perspective. After that we investigate how to generalise Carlen and Maas' result to countable infinite Hilbert spaces.

To obtain the final result we have split this dissertation into multiple parts. In Chapter 1 we introduce the framework of quantum mechanics and Quantum Markov Semigroups (QMS)

with their generators. Here, some key theorems and notions related to generators are stated and proven to introduce the reader to the background required for the rest of the thesis. Furthermore, in Chapter 2 we consider two important theorems: the Kadison-Schwarz inequality and the Russo-Dye theorem. These two theorems are then used to derive the relation between dissipative operators and generators of QMS. Additionally, in Chapter 3 we prove the Lindblad equation from both the mathematical and physical perspective. For the mathematical perspective we follow the original paper as published by Lindblad [16], while for the physical perspective we do not consider the original paper, but rather a newer and cleaner version of the derivation as shown by Manzano [18]. Lastly, in Chapter 4 we introduce a new class of operators called the Hilbert-Schmidt operators with the Hilbert-Schmidt inner product. This inner product is crucial in making the trace class operators a space with Hilbert space structure. Furthermore, we introduce the modular automorphisms group. Finally, we use the trace class operators with the Hilbert-Schmidt inner product and the Hilbert-Schmidt operators to prove the simplified form of the Lindblad equation under the assumption that the generator commutes with the modular automorphisms group.

NOMENCLATURE

The following list describes a set of symbols and notations used in the dissertation.

Mathematical operations

- $\langle \cdot, \cdot \rangle$ The inner product.
- $\| \cdot \|$ The norm.
- \oplus The direct sum.
- \otimes The tensor product.
- $\text{Tr}(\cdot)$ The trace.
- $\text{Tr}_B(\cdot)$ The partial trace over subspace B.
- $*$ The adjoint, for finite dimensional matrices $X^* = \overline{X}^T$.

Number theory

- \mathbb{N} The natural numbers, $\{1, 2, 3, \dots\}$.
- \mathbb{R} The real numbers.
- \mathbb{C} The complex numbers, $\{a + bi : a, b \in \mathbb{R}\}$.

Spaces

- $M_n(\mathbb{C})$ The $n \times n$ square matrices over the complex numbers.
- \mathcal{H} A Hilbert space.
- $\mathcal{L}(\mathcal{H})$ The linear operators on Hilbert space \mathcal{H} .
- $B(\mathcal{H})$ The bounded linear operators on a Hilbert space \mathcal{H} .
- $\mathcal{L}_1(\mathcal{H})$ The trace class operators on a Hilbert space \mathcal{H} .
- $\mathcal{L}_2(\mathcal{H})$ The Hilbert-Schmidt operators on a Hilbert space \mathcal{H} .
- $\mathcal{L}_3(\mathcal{H})$ $\mathcal{L}_2(\mathcal{H})' \oplus \{\lambda I : \lambda \in \mathbb{C}\}$, with $\mathcal{L}_2(\mathcal{H})'$ the trace class operators with a special inner product.
- $\mathcal{L}_4(\mathcal{L}_3(\mathcal{H}))$ $\mathcal{L}_2(\mathcal{L}_3(\mathcal{H})) \oplus \{\lambda I : \lambda \in \mathbb{C}\}$ with a special inner product.

Notation

- v Small letters denote vectors.
- X Capital letters denote operators.

1

NOTIONS ON QUANTUM MECHANICS AND MATHEMATICAL PRELIMINARIES

In this chapter we introduce several important concepts from quantum mechanics. Furthermore, concepts and theorems related to the theory of completely positive maps are presented. Lastly, semigroups and their generators are discussed. All of these are fundamental notions, meaning that a more thorough exploration of particular topics can be found in the literature that will be referred to throughout the chapter.

1.1. DENSITY OPERATORS

In this section we introduce density operators through a discussion about quantum states and ensembles. We also briefly mention the postulates that form the basis of quantum mechanics, whilst also explaining the difference between the Heisenberg and Schrödinger picture of quantum physics.

1.1.1. VECTOR NOTATION AND THE DENSITY OPERATOR

Definition 1.1. A complete, normed vector space \mathcal{H} endowed with an inner product $\langle \cdot, \cdot \rangle : \mathcal{H} \times \mathcal{H} \rightarrow \mathbb{C}$ is called a Hilbert space.

Usually we will let our Hilbert space \mathcal{H} be given by \mathbb{C}^n . One of the most common examples of this particular Hilbert space is for instance the spin state of an electron which is represented as a vector in \mathbb{C}^2 . We have the following identification for states of a system: given a vector $\psi \in \mathcal{H}$, if $\|\psi\| = 1$, then the vector is a unit vector. Unit vectors in a Hilbert space represent states of the underlying physical system. Now that we have defined a vector, we can define its adjoint in the adjoint vector space \mathcal{H}^* .

Definition 1.2. The adjoint of a vector $\psi \in \mathcal{H}$ is a linear functional $\psi^* : \mathcal{H} \rightarrow \mathbb{C}$ thus $\psi^* \in \mathcal{H}^*$, defined by:

$$\psi^*(\phi) := \langle \psi, \phi \rangle \quad \forall \phi \in \mathcal{H}. \quad (1.1)$$

This notation is important, because it will allow us to represent the vectors and adjoint vectors in a mathematical way. Next, we continue with some important notions.

Definition 1.3. A basis $\{e_i\}_{i=1}^n$ for \mathcal{H} is orthonormal if

$$\sum_{i=1}^n e_i e_i^* = I \quad \text{and} \quad \|e_i\| = 1 \quad \forall i = 1, \dots, n. \quad (1.2)$$

In this equation I is the identity operator.

An orthonormal basis gives us the following natural representation of a vector in \mathcal{H} :

$$\psi = \sum_i \langle \psi, e_i \rangle e_i. \quad (1.3)$$

Furthermore, this notation allows us to define an important object: the density operator.

Definition 1.4. Given an ensemble of states $\{\psi_i\}$ with observation probabilities $\{p_i : p_i$ the probability to observe state $\psi_i\}$ the density operator is defined as

$$\rho = \sum_i p_i \psi_i \psi_i^*. \quad (1.4)$$

A natural consequence of this definition is the following.

Definition 1.5. A state is called pure if the density operator ρ can be written as $\rho = \psi \psi^*$ for some $\psi \in \mathcal{H}$ with $\|\psi\| = 1$.

The density operator encodes the essential information about the underlying statistical ensemble of states in the system. Which states can be observed and with what probability.

1.1.2. POSTULATES OF QUANTUM MECHANICS

To continue our discussion of quantum mechanics, we now consider the postulates related to the quantum mechanics. These postulates form the framework in which the rest of quantum mechanics is built. To define the proper postulates we will follow the definitions of Nielsen and Chuang [21] (pages 102-103).

Postulate 1. The state space associated to an isolated physical system can be represented by a complex Hilbert space \mathcal{H} . The system is completely described by its density operator, which is a positive operator $\rho > 0$ with $\text{Tr}(\rho) = 1$.

The notation $\rho > 0$ represents the following fact: for any $x \in \mathcal{H}$ with $x \neq 0$ we have that $\langle x, \rho x \rangle > 0$, this notation will be used from now on. To continue our discussion on the postulates of quantum mechanics, we now consider dynamics. To describe the dynamics of a single state system the Schrödinger equation is used, however in the case of density operators we have the following postulate:

Postulate 2. The evolution of a closed quantum system is described by a unitary transformation. That is, the state ρ of the system at time t_1 is related to the state of the system at time t_2 by the unitary operator U , which depends only on t_1, t_2 ,

$$\rho' = U \rho U^*. \quad (1.5)$$

In this definition the $*$ denotes the conjugate transpose of the operator. If the system is described by a Hamiltonian H and H is time independent, the operators U can easily be derived from the Schrödinger equation to be given by $U(t) = e^{-iHt/\hbar}$. Now that the dynamics of the system have been described, we move on to measuring the system.

Postulate 3. Quantum measurements are described by a collection of measurement operators $\{M_i\}_{i=\text{one of the outcomes}}$. Given that the system is in state ρ immediately before the measurement, we have that the system right after the measurement is in state

$$\frac{M_i \rho M_i^*}{\text{Tr}(M_i^* M_i \rho)}. \quad (1.6)$$

here the state has been normalised by the probability p_i that we observe state i . This probability is given by

$$p_i = \text{Tr}(M_i \rho M_i^*) = \text{Tr}(M_i^* M_i \rho). \quad (1.7)$$

where the permutation property of the trace has been used, i.e. $\text{Tr}(AB) = \text{Tr}(BA)$ which can be shown by a rather trivial computation. The given measurement operators must satisfy the completeness equation to be called a set of measurement operators:

$$\sum_{i=1}^n M_i^* M_i = I. \quad (1.8)$$

The last postulate considers combining physical systems and describing the joint state.

Postulate 4. The state space of a composite physical system is the tensor product of the state spaces of the component physical systems. Moreover, if we have systems numbered 1 through n , and the system number i is prepared in the state ρ_i then the joint state of the total system is given by $\rho_1 \otimes \cdots \otimes \rho_n$.

If the reader is not familiar with tensor products, we refer to Appendix A. Furthermore, the postulate on combining physical systems is important because it gives us the opportunity to combine or separate (if possible) physical systems. This separation can be achieved by tracing out the system we are not interested in. This is done using the partial trace operation.

Definition 1.6. Let systems A and B be described by the density operators σ and ν respectively. The combined system is then represented by density operator $\rho = \sigma \otimes \nu$. The partial trace over system B is then defined as $\text{Tr}_B : A \otimes B \rightarrow A$ given by

$$\text{Tr}_B(\rho) = \text{Tr}_B(\sigma \otimes \nu) = \sigma \text{Tr}_B(\nu) = \sigma. \quad (1.9)$$

This equation can be extended linearly for any convex combinations of ρ 's representing states in the systems.

1.1.3. DIFFERENT PICTURES OF QUANTUM MECHANICS

In quantum physics there are two views concerning the evolution of quantum systems. Looking back at the previous part, we note that the postulates of Nielsen and Chuang are formulated in the Schrödinger picture. This way of viewing quantum mechanics implies that states

are evolving with time and operators are time-independent. The time dependence of the states in the system can be seen in equation 1.5. Additionally, notice that the measurement operators are independent of time i.e. the observables do not change in time. This description is powerful, because it lets us map density matrices to density matrices using trace preserving completely positive maps. However, as is often the case in mathematics and physics, another description could be more powerful. The other description in this case is given by the Heisenberg picture, which is concerned with unital completely positive maps. Notice that unital and trace preserving are switched when switching between the two descriptions. In the Heisenberg picture states remain fixed, but operators change with time. This is physically more appealing, because of the time dependence of quantities like momentum and position. Hence, there are advantages to both pictures, but it actually turns out that the Heisenberg description is much more powerful because of some key theorems. Furthermore, these two pictures actually turn out to be each others dual. To fully understand why this is the case we require the language of completely positive maps, which is covered in the next section.

1.2. UNITAL COMPLETELY POSITIVE MAPS

We have introduced the fundamental concepts and notations of quantum mechanics. However, to properly understand and derive the Lindblad Master equation we need to understand the language of unital completely positive maps. We will do this by following the notes by Paulsen [12] (pages 3-30).

1.2.1. COMPLETE POSITIVITY

This part is used to introduce some important definitions concerning positivity and to introduce some useful notation.

Notation 1.7. For any matrix M we will also denote the matrix as (M_{ij}) for convenience.

Another important notation is the way we denote the linear operators on a space.

Notation 1.8. The linear operators on a Hilbert space \mathcal{H} are denoted by $\mathcal{L}(\mathcal{H})$.

In this thesis we will restrict our discussion to finite dimensional Hilbert spaces until the last chapter. Hence, until we explicitly state it, \mathcal{H} is finite. We now introduce the notion of complete positivity. By defining the following

Definition 1.9. For any linear map $\Phi : \mathcal{L}(\mathcal{H}_1) \rightarrow \mathcal{L}(\mathcal{H}_2)$, we define the map $\Phi^{(n)} : M_n(\mathcal{L}(\mathcal{H}_1)) \rightarrow M_n(\mathcal{L}(\mathcal{H}_2))$ by $\Phi^{(n)}((W_{ij})) := (\Phi(W_{ij}))$ for a matrix $(W_{ij}) \in \mathcal{L}(\mathcal{H}_1)$.

Definition 1.10. A linear map $\Phi : \mathcal{L}(\mathcal{H}_1) \rightarrow \mathcal{L}(\mathcal{H}_2)$ is called n -positive if for any $(W_{ij}) \in M_n(\mathcal{L}(\mathcal{H}_1))$ with $(W_{ij}) \geq 0$ we have that $(\Phi(W_{ij})) \geq 0$. We say that Φ is completely positive (CP) if Φ is n -positive $\forall n \in \mathbb{N}$ we then also write that $\Phi \in \text{CP}(\mathcal{L}(\mathcal{H}_1), \mathcal{L}(\mathcal{H}_2))$. If $\mathcal{L}(\mathcal{H}_1) = \mathcal{L}(\mathcal{H}_2)$ we simply write $\text{CP}(\mathcal{L}(\mathcal{H}_1))$. Additionally, if Φ also preserves the identity element, i.e. if I is the identity in $\mathcal{L}(\mathcal{H}_1)$, then $\Phi(I)$ is the identity in $\mathcal{L}(\mathcal{H}_2)$, the map Φ is then called a unital completely positive map or UCP.

1.2.2. CHOI-KRAUS THEOREM

The definitions in the preceding section may seem very abstract at first, however Choi and Kraus proved a theorem which states that there is an easier identification of CP maps. We

state the theorem and its proof. Additionally, we also discuss the Stinespring dilation theorem. Furthermore, this identification will show a nice correspondence between measurement operators and the UCP maps.

Theorem 1.11 (Choi-Kraus Representation). Let $\Phi : M_n \rightarrow M_d$ be a linear map. Then the following are equivalent.

- i) Φ is completely positive
- ii) There exist $B_1, \dots, B_K \in M_{d,n}$, such that $\Phi(X) = \sum_{k=1}^K B_k X B_k^*$ for all $X \in M_n$.

Proof. We will first proof the converse. To this end, let $m \in \mathbb{N}$ arbitrary and let $(X_{ij}) \in M_m(M_n)$ be positive. Then

$$\Phi^{(m)}((X_{ij})) = (\Phi(X_{ij})) = \left(\sum_{k=1}^K B_k X_{ij} B_k^* \right) = \sum_{k=1}^K (B_k X_{ij} B_k^*) \geq 0. \quad (1.10)$$

In this equation the last equality follows from the linearity of matrix addition. The last inequality follows from the fact that the sum of positive semidefinite matrices is positive semidefinite. Hence, Φ is CP.

We will now prove the implication. Let $z \in \mathbb{N}$ be arbitrary and let $A := (E_{ij}) \in M_z(M_d)$, where the E_{ij} are the matrices with zeros everywhere except for $e_{i,j} := 1$. Then proceeding as follows

$$Q^* = (E_{ij})^* = (E_{ji}^*) = (E_{ij}) = Q. \quad (1.11)$$

This implies that Q is an Hermitian matrix. Furthermore,

$$Q^2 = \left(\sum_{k=1}^n E_{ik} E_{kj} \right) = \left(\sum_{k=1}^n E_{ij} \right) = (nE_{ij}) = nQ. \quad (1.12)$$

Where again we have again used linearity and the fact that the E_{ij} are identically zero everywhere except on element $e_{i,j} = 1$. We now want to find the eigenvalues λ of Q . Hence, consider that for all eigenvectors x of Q we have that

$$\lambda^2 x = Q^2 x = nQx = n\lambda x \iff \lambda \in \{0, n\}. \quad (1.13)$$

Since we now have that all $\lambda \geq 0 \implies Q \geq 0$. Thus, Q is a positive semidefinite matrix. By n -positivity of Φ this implies that $\Phi^{(z)}(Q) \geq 0$. This is an $zd \times zd$ matrix. Therefore, there exist vectors $v_1, \dots, v_K \in \mathbb{C}^{zd}$ such that $\Phi^{(z)}(Q) = \sum_{k=1}^K v_k v_k^*$ by the Spectral Theorem of Linear Algebra. Here we have taken the eigenvalues into the vectors.

Since

$$v_k \in \mathbb{C}^{zd} \implies v_k = \begin{pmatrix} h_1^k \\ \vdots \\ h_z^k \end{pmatrix}, \text{ with } h_i^k \in \mathbb{C}^d \quad \forall i \in \{1, \dots, z\}. \quad (1.14)$$

Note that π is usually called a representation. Additionally, the fact that π is a $*$ -map implies that $\pi(X)^* = \pi(X^*)$ for all $X \in B(\mathcal{H})$. It should be noted that the proof is well known and therefore we will not prove this theorem. However, for the interested reader we recommend Stinespring [24] and Caspers [7] (pages 44-45). The theorem itself is required to prove the final part of the Lindblad derivation in Chapter 3.

We continue on with the Choi-Kraus decomposition, by using this theorem we can prove the following identification of trace preserving completely positive maps. If a map is TPCP, then these are the measurement operators as mentioned earlier. Before we can prove this corollary, we need the following lemma.

Lemma 1.13. Given $Y \in M_n$ then $\text{Tr}(XY) = \text{Tr}(X)$ for all $X \in M_n$ if and only if $Y = I_n$.

The proof is rather trivial and shall be omitted here. We continue on with the following result.

Corollary 1.14. Let $\Phi: M_n \rightarrow M_d$ be a linear map. Then Φ is a TPCP map if and only if $\Phi(X) = \sum_{k=1}^K B_k X B_k^*$ with $\sum_{k=1}^K B_k^* B_k = I_d$.

Proof. We begin with the direct implication. By the Choi-Kraus theorem there are B_k such that $\Phi(X) = \sum_{k=1}^K B_k X B_k^*$. Then we obtain the following

$$\begin{aligned} \text{Tr}(\Phi(X)) &= \text{Tr}\left(\sum_{k=1}^K B_k X B_k^*\right) \\ &= \sum_{k=1}^K \text{Tr}(B_k X B_k^*) \\ &= \sum_{k=1}^K \text{Tr}(X B_k^* B_k) \\ &= \text{Tr}\left(X \sum_{k=1}^K B_k^* B_k\right). \end{aligned} \tag{1.18}$$

Using the previous lemma and setting $\sum_{k=1}^K B_k^* B_k = Y$ implies that $\sum_{k=1}^K B_k^* B_k = Y = I_n$. For the converse, we have that by Choi-Kraus Φ is a CP map. Taking the trace yields again the above equation. Notice that the last term in the equality evaluates to $\text{Tr}(X)$, if $\sum_{k=1}^K B_k^* B_k = I_d$. ■

As mentioned in subsection 1.1.3 these TPCP maps are part of the Schrödinger picture. To derive the duality between the Schrödinger picture and the Heisenberg picture of UCP maps, we require the following definition and proposition from Caspers' notes [7] (page 68).

Definition 1.15. Let $\Phi: M_n(\mathbb{C}) \rightarrow M_n(\mathbb{C})$ be any linear map. Then we set $\Phi^*: M_n(\mathbb{C}) \rightarrow M_n(\mathbb{C})$ as the unique map determined by

$$\text{Tr}(\Phi^*(X)Y) = \text{Tr}(X\Phi(Y)), \quad \forall X, Y \in M_n(\mathbb{C}). \tag{1.19}$$

We can then formulate the following proposition showing the equivalence

Proposition 1.16. In the setting of the previous definition we have that Φ is trace preserving (respectively unital) if and only if Φ^* is unital (respectively trace preserving).

Proof. Suppose that Φ is trace preserving. Then let $X, Y \in M_n(\mathbb{C})$ which implies

$$\mathrm{Tr}(\Phi^*(I)Y) = \mathrm{Tr}(I\Phi(Y)) = \mathrm{Tr}(Y). \quad (1.20)$$

Therefore, $\Phi^*(I) = I$. Conversely, suppose that Φ^* is unital. Then again let $X, Y \in M_n(\mathbb{C})$, which implies

$$\mathrm{Tr}(\Phi(Y)) = \mathrm{Tr}(I\Phi(Y)) = \mathrm{Tr}(\Phi^*(I)Y) = \mathrm{Tr}(Y). \quad (1.21)$$

which concludes the proof. \blacksquare

This proposition shows that we can use either UCP maps or TPCP maps. Hence, we can use both the Heisenberg and Schrödinger picture. As mentioned before, because of ease of use, we prefer the Heisenberg picture.

1.3. SEMIGROUPS AND GENERATORS

In this section we will discuss the notion of dynamical semigroups and their generators. We will first define a dynamical semigroup and then derive some elementary and useful results. Additionally, the Hille-Yosida theorem concerning the existence of generators is discussed.

1.3.1. SEMIGROUPS

In this part we will define a semigroup and the regular setting in which we will be working.

Definition 1.17. The set of bounded linear operators on a Hilbert space \mathcal{H} denoted by $B(\mathcal{H})$ is given by all operators which have a finite operator norm. i.e.

$$B(\mathcal{H}) = \{X : \|X\| < \infty, X \in \mathcal{L}(\mathcal{H})\}. \quad (1.22)$$

In this equation the norm is given by

$$\|X\| = \sup_{\psi \in \mathcal{H} \setminus \{0\}} \frac{\|X\psi\|_{\mathcal{H}}}{\|\psi\|_{\mathcal{H}}}. \quad (1.23)$$

where the second norm is the norm on \mathcal{H} induced by the inner product, defined as

$$\|\psi\|_{\mathcal{H}} = \sqrt{\langle \psi, \psi \rangle}. \quad (1.24)$$

In the rest of the paper it will always be clear which norm will be used. Hence, we will drop the \mathcal{H} . However, for this definition we noted it explicitly for clarity. Additionally, it should be noted that the general definition of the operator norm on a Banach space is given by the following definition

Definition 1.18. Let $X : A \rightarrow B$ for A, B Banach spaces. Then the norm on X is defined as

$$\|X\| = \sup_{\xi \in A} \frac{\|X\xi\|}{\|\xi\|}. \quad (1.25)$$

To properly define the axioms that make up a semigroup, we need to define what kind of continuity and convergence we require. However, in the case of complex valued finite dimensional matrices the different topologies are all equivalent, so in this case the type of topology does not matter. Nevertheless, to keep ourselves aligned with the derivation of Lindblad we will require the following topologies aside from the regular norm topology.

Definition 1.19. The strong operator topology on $B(\mathcal{H})$ often abbreviated as SOT is the topology with a subbasis given by

$$O(X, x, \varepsilon) = \{A \in B(\mathcal{H}) : \|(A - X)x\| < \varepsilon\}. \quad (1.26)$$

We have that $A_n \rightarrow X$ in the SOT if and only if for all $x \in \mathcal{H}$ $\|A_n x - Xx\| \rightarrow 0$ i.e. $A_n x \rightarrow Xx$ strongly.

Definition 1.20. The weak operator topology on $B(\mathcal{H})$ often abbreviated as WOT is the topology with a subbasis given by

$$O(X, x, y, \varepsilon) = \{A \in B(\mathcal{H}) : \langle (A - X)x, y \rangle < \varepsilon\}. \quad (1.27)$$

Now $A_n \rightarrow X$ in the WOT if and only if for all $x \in \mathcal{H}$ and $y \in \mathcal{H}$ $\langle (A_n - X)x, y \rangle \rightarrow 0$ i.e. $A_n x \rightarrow Xx$ weakly.

It turns out that the weak operator topology is weaker than the strong operator topology, which is again weaker than the norm topology. Lastly, we define the weak* or ultraweak topology, which is the topology induced by the dual space. We will begin by defining the dual of the $B(\mathcal{H})$. To this end consider the trace class operators.

Definition 1.21. A bounded operator $X \in B(\mathcal{H})$ is called trace class if its modulus $|X| = |X^* X|^{1/2}$ has finite trace. We denote the entire set of trace class operators with $\mathcal{L}_1(\mathcal{H})$.

In this definition it should be noted that in functional calculus the square root f of a functional g is defined as $g(x) = f(f(x))$, i.e. composition, for all x in the domain of g . Furthermore, it is a well known fact from functional calculus that every positive operator X has a unique square root S such that $S^2 = X$, for the interested reader we would recommend Van Neervens notes [26] (pages 266-269). Additionally, an important fact about $\mathcal{L}_1(\mathcal{H})$ is that it is a Banach space, with norm $\|X\| = \text{Tr}(|X|)$. Furthermore, there is a duality between $B(\mathcal{H})$ and $\mathcal{L}_1(\mathcal{H})$. More precisely we have that $B(\mathcal{H}) \simeq \mathcal{L}_1(\mathcal{H})^*$, this is a well known fact from functional analysis, which can be found in for instance Murphy [19] (pages 125-126). This dual space of trace class operators induces a topology on $B(\mathcal{H})$ called the weak* topology defined in the following definition.

Definition 1.22. Let $(X_n)_{n=1}^\infty \subset B(\mathcal{H})$ converges weak* to $X \in B(\mathcal{H})$ if

$$\text{Tr}(XY) = \lim_{n \rightarrow \infty} \text{Tr}(X_n Y) \quad \text{for all } Y \in \mathcal{L}_1(\mathcal{H}). \quad (1.28)$$

This implies that the topology is generated by the semi-norms

$$X \mapsto |\text{Tr}(XY)| \quad Y \in \mathcal{L}_1(\mathcal{H}). \quad (1.29)$$

It should be noted that the weak* topology is actually stronger than the WOT, which therefore has a bit of a confusing naming scheme. Additionally, we have a specific requirement regarding the strong operator topology.

Definition 1.23. An operator $\Phi : B(\mathcal{H}) \rightarrow B(\mathcal{H})$ is called normal if it is strongly continuous on the unit ball in $B(\mathcal{H})$.

Kossawaki [14] defined the quantum dynamical semigroup as follows

Definition 1.24. $\mathcal{P}(\Phi) = \{\Phi_t : t \geq 0\}$ of linear endomorphisms on $B(\mathcal{H})$ is called a quantum dynamical semigroup if

- i) Φ_t is positive.
- ii) Φ_t is unital.
- iii) $\Phi_t \cdot \Phi_s = \Phi_{s+t}$.
- iv) $\lim_{t \rightarrow 0^+} \|\Phi_t - I\| = 0$. I.e. Φ_t is norm continuous.
- v) Φ_t is normal.

1.3.2. INFINITESIMAL GENERATORS OF DYNAMICAL SEMIGROUPS

In this section we will define the infinitesimal generator of a quantum dynamical semigroup and derive several key theorems and results. These results include the denseness of the generator in the range of the semigroup. Furthermore, we will show that the exponential formula of the generator yields the entire semigroup. To define these concepts we will use some proofs of Hille and Philips [13] (pages 306-308 and 310-312).

Let us first define a generator.

Definition 1.25. Given a quantum dynamical semigroup $\mathcal{P}(\Phi) = \{\Phi_t : t \geq 0\}$ defined on Hilbert space \mathcal{H} . We define the infinitesimal generator L as $\eta \rightarrow 0^+$ of

$$L_\eta X = \frac{1}{\eta} [\Phi_\eta - I] X \quad \forall X \in B(\mathcal{H}). \quad (1.30)$$

We say that $X \in D(L)$ or X is in the domain of L if the above defined limit exists. Furthermore, by the assumption that $\mathcal{P}(\Phi)$ is actually norm continuous, we know that the generator is a bounded linear mapping. This implies that we can replace our definition with the following requirement

$$\lim_{t \rightarrow 0^+} \left\| L - \frac{(\Phi_t - I)}{t} \right\| = 0 \quad (1.31)$$

Currently, the definition does not tell us why L is called a generator. This will become apparent after we have derived the exponential formula. However, to achieve this result we first prove that $D(L)$ is dense in $\{\Phi_t[B(\mathcal{H})] : t \geq 0\}$, here $\Phi_t[B(\mathcal{H})]$ represents the image of $B(\mathcal{H})$ under Φ_t .

Theorem 1.26 (Hille-Yosida). If Φ_t is strongly continuous and L is the infinitesimal generator of Φ_t then $D(L)$ is dense in $\{\Phi_t[B(\mathcal{H})] : t \geq 0\} = B(\mathcal{H})$.

Proof. We need to prove that $\forall X \in B(\mathcal{H})$, there exists a sequence $\{X_n\}_{n=1}^\infty \subset D(L)$ such that $X_n \rightarrow X$ as $n \rightarrow \infty$. To this end, let $X \in B(\mathcal{H})$. In this case there exists a $t \geq 0$ and a $Y \in B(\mathcal{H})$ such that $\Phi_t Y = X$. Now let α, β be given as $\alpha < \beta = t$. Claim: the element given as

$$x_{\alpha, \beta} = \int_\alpha^\beta \Phi_\tau Y d\tau \quad (1.32)$$

is part of $D(L)$. We have that

$$L_\eta x_{\alpha, \beta} = \frac{1}{\eta} \int_\alpha^\beta (\Phi_\eta - I) \Phi_\tau Y d\tau$$

$$\begin{aligned}
&= \frac{1}{\eta} \int_{\alpha}^{\beta} (\Phi_{\eta+\tau} - \Phi_{\tau}) Y d\tau \\
&= \frac{1}{\eta} \int_{\alpha+\eta}^{\beta+\eta} \Phi_{\sigma} Y d\sigma - \frac{1}{\eta} \int_{\alpha}^{\beta} \Phi_{\sigma} Y d\sigma \\
&= \frac{1}{\eta} \int_{\beta}^{\beta+\eta} \Phi_{\sigma} Y d\sigma - \frac{1}{\eta} \int_{\alpha}^{\alpha+\eta} \Phi_{\sigma} Y d\sigma \\
&\rightarrow [\Phi_{\beta} - \Phi_{\alpha}] Y \quad \eta \rightarrow 0^+.
\end{aligned}$$

Where the last convergence is convergence in norm. This can be seen as follows let $\epsilon > 0$ then by strong continuity of Φ_t there exists a δ such that if $|\sigma - \beta| < \delta$ we have that $\|(\Phi_{\sigma} - \Phi_{\beta})Y\| < \epsilon$. Using this fact notice that

$$\begin{aligned}
\left\| \frac{1}{\eta} \int_{\beta}^{\beta+\eta} \Phi_{\sigma} Y d\sigma - \Phi_{\beta} Y \right\| &= \left\| \frac{1}{\eta} \int_{\beta}^{\beta+\eta} (\Phi_{\sigma} - \Phi_{\beta}) Y d\sigma \right\| \\
&\leq \frac{1}{\eta} \int_{\beta}^{\beta+\eta} \|(\Phi_{\sigma} - \Phi_{\beta})Y\| d\sigma \\
&< \epsilon.
\end{aligned}$$

Hence, $x_{\alpha,\beta} \in D(L)$. Now consider the case with $\alpha < \beta = t$, then

$$\frac{x_{\alpha,t}}{t-\alpha} = \frac{1}{t-\alpha} \int_{\alpha}^t \Phi_{\tau} Y d\tau \rightarrow \Phi_t Y = X \quad \text{as } \alpha \rightarrow t. \quad (1.33)$$

We have thus found the sequence converging to X . Since this X was arbitrary we have that $\overline{D(L)} = B(\mathcal{H})$. \blacksquare

This denseness was part of the proof provided by Hille and Yosida about infinitesimal generators and is required to properly use L as the generator of the semigroup. Moving on to the following lemma.

Lemma 1.27. If Φ_t is strongly continuous for all $t \geq 0$, then for all $X \in D(L)$ we have

$$\frac{d\Phi_t}{dt} X = L\Phi_t X = \Phi_t L X. \quad (1.34)$$

I.e. the generator and the operators commute. The proof is easy to see by using the definition of the derivative and L_{η} . This important lemma allows us to state the following theorem.

Theorem 1.28. If $\|\Phi_t\| \leq 1$ i.e. $\mathcal{P}(\Phi)$ is a contraction semigroup and Φ_t is strongly continuous then for all $X \in B(\mathcal{H})$

$$\lim_{\eta \rightarrow 0^+} e^{tL_{\eta}} X = \Phi_t X. \quad (1.35)$$

Where we defined the operator exponential for any operator X to be given by

$$e^X = I + X + \frac{1}{2}X^2 + \dots + \frac{1}{k!}X^k + \dots \quad (1.36)$$

Proof. Notice that

$$e^{tL_\eta} = e^{t \frac{\Phi_\eta - I}{\eta}} = e^{-\frac{t}{\eta}} e^{\frac{t\Phi_\eta}{\eta}}. \quad (1.37)$$

Furthermore, one could notice then that

$$\|e^{tL_\eta}\| \leq e^{-\frac{t}{\eta}} e^{\|\Phi_\eta\| \frac{t}{\eta}} = e^{-\frac{t}{\eta}} e^{\frac{t}{\eta}} = 1. \quad (1.38)$$

We know that $e^{(t-\tau)L_\eta} X$ is a differentiable function if $X \in D(L)$. Additionally, it can be deduced that

$$\frac{d}{d\tau} (e^{(t-\tau)L_\eta} \Phi_\tau X) = e^{(t-\tau)L_\eta} \left(\frac{d\Phi_\tau}{d\tau} X - L_\eta \Phi_\tau X \right) = e^{(t-\tau)L_\eta} (\Phi_\tau LX - L_\eta \Phi_\tau X). \quad (1.39)$$

Here, we used lemma 1.27 to switch the derivative with $\Phi_\tau L$. Then we use the following identification

$$\Phi_t X - e^{tL_\eta} X = \int_0^t \frac{d}{d\tau} (e^{(t-\tau)L_\eta} \Phi_\tau X) d\tau. \quad (1.40)$$

Which yields

$$\begin{aligned} \left\| \int_0^t \frac{d}{d\tau} (e^{(t-\tau)L_\eta} \Phi_\tau X) d\tau \right\| &\leq \int_0^t \|e^{(t-\tau)L_\eta}\| \|LX - L_\eta X\| \|\Phi_\tau\| d\tau \\ &\leq \int_0^t \|LX - L_\eta X\| d\tau \\ &= t \|LX - L_\eta X\| \rightarrow 0 \text{ as } \eta \rightarrow 0^+. \end{aligned} \quad (1.41)$$

This result is true for any $X \in D(L)$, but also note that $\lim_{t \rightarrow 0^+} \Phi_t X = X$ by the requirements of a semigroup. Which gives us $\overline{B(\mathcal{H})} = B(\mathcal{H})$. By theorem 1.26 we know that $\overline{D(L)} = B(\mathcal{H})$. Hence, this formula holds for all $X \in B(\mathcal{H})$. \blacksquare

This proof shows us why L is called the generator of $\mathcal{P}(\Phi)$, it gives us the natural identification $\exp(tL)X = \Phi_t X$. This is useful, because it allows us to work with generators instead of unwieldy infinite sets. Furthermore, for L to generate the norm continuous semigroup as defined by in definition 1.24 we require L to be ultraweakly or weak* continuous, which is a result we will not prove, but is required in later chapters.

2

DISSIPATIVE OPERATORS

In this chapter we consider dissipative operators. These are discussed in two parts. First, we consider two key theorems: The Kadison-Schwarz inequality and the Russo-Dye theorem. Initially we look at the Kadison-Schwarz inequality, which is a generalisation of the Cauchy-Schwarz inequality for 2-positive maps. After this we state and prove the Russo-Dye theorem, which lets us rewrite the supremum of the operator norm into a supremum only depended on unitary elements. In the second part of the chapter we both define completely dissipative operators and show the equivalence of Kadison-Schwarz and Russo-Dye for contraction semigroups. Lastly, we discuss a theorem concerning the fact that the dissipation function determines the generator of a group of CP maps up to a Hamiltonian. This shows a physical equivalence to the mathematics proposed in this chapter.

2.1. TWO KEY THEOREMS

In this section we discuss the Kadison-Schwarz inequality and the Russo-Dye theorem. These two results are important and well known results in the theory of linear maps and in our case specifically the theory of completely positive maps.

2.1.1. KADISON-SCHWARZ INEQUALITY

The Kadison-Schwarz inequality will play a key role in the derivation of the Lindblad equation later on, which is why it is treated here.

We start off by noting that $M_n(\mathbb{C})$ has a unitary element, namely the identity operator I . Using this fact we can derive the Kadison-Schwarz inequality.

Theorem 2.1 (Kadison-Schwarz). Let $\Phi : M_n(\mathbb{C}) \rightarrow M_n(\mathbb{C})$ be 2-positive, then

$$\Phi(X^*)\Phi(X) \leq \|\Phi(I)\|\Phi(X^*X), \quad \forall X \in M_n(\mathbb{C}). \quad (2.1)$$

Proof. By rescaling, we can assume that $\|\Phi(I)\| = 1$. Furthermore, let $X \in M_n(\mathbb{C})$ after which we consider the following matrix:

$$K = \begin{pmatrix} I & X \\ 0 & 0 \end{pmatrix}.$$

We then have that K^*K is positive

$$K^*K = \begin{pmatrix} I & X \\ X^* & X^*X \end{pmatrix} \geq 0. \quad (2.2)$$

Using this matrix and setting I_2 to be the identity matrix of size 2×2 . We then have

$$0 \leq (\Phi \otimes I_2)(K^*K) = \begin{pmatrix} \Phi(I) & \Phi(X) \\ \Phi(X^*) & \Phi(X^*X) \end{pmatrix} \leq \begin{pmatrix} I & \Phi(X) \\ \Phi(X^*) & \Phi(X^*X) \end{pmatrix}. \quad (2.3)$$

The last inequality simply states that $\langle \Phi(I)\xi, \xi \rangle \leq \langle \xi, \xi \rangle = \|\xi\|^2$. This can be proved as follows: first we can, without loss of generality, assume that the vectors have unit length. We then have

$$\langle \Phi(I)\xi, \xi \rangle \leq \sup_{\xi, \eta \in \mathcal{H}} |\langle \Phi(I)\xi, \eta \rangle| \leq \|\Phi(I)\| \|\xi\| \|\eta\| = \|\Phi(I)\| = 1. \quad (2.4)$$

In this equation we used the Cauchy-Schwarz inequality to derive an upper bound on the absolute value.

Employing the fact that the last matrix is a positive matrix yields that it must also be positive when taking the inner product with the vector given as $(\Phi(X)^* \quad -1)^*$. This yields

$$0 \leq (\Phi(X)^* \quad -1) \begin{pmatrix} I & \Phi(X) \\ \Phi(X^*) & \Phi(X^*X) \end{pmatrix} \begin{pmatrix} \Phi(X) \\ -1 \end{pmatrix} = \Phi(X^*X) - \Phi(X^*)\Phi(X). \quad (2.5)$$

Which completes the proof. ■

The Kadison-Schwarz derivation initially required Φ to be CP. However, in 1972, Choi [8] simplified the result to only require 2-positivity, which is the proof shown above. Furthermore, Stinespring [24] proved that if the matrix algebra is abelian then every positive map is completely positive. This means that the Kadison-Schwarz inequality also holds if Φ is positive and we only consider the elements with $XX^* = X^*X$, which are usually called normal elements.

2.1.2. RUSSO-DYE THEOREM

In this part we cover key results from Russo and Dye, which will mainly focus on simplifying the operator norm defined in equation 1.23 and having another useful identification of positivity, which is required later on.

Russo and Dye [22] proved in their paper that the convex hull of the unitary operators of $B(\mathcal{H})$ are dense in the unit sphere of $B(\mathcal{H})$. This result also yields that any operator $X \in B(\mathcal{H})$ has a decomposition in terms of unitary operators, since we can span the entire space $B(\mathcal{H})$ by considering linear combinations of the unitary elements. In particular, any operator can be written as a linear combination of four unitary operators. We will use this fact to derive the Russo-Dye theorem. However, to start of we first define the following norm.

Definition 2.2. Suppose $X \in M_n(\mathbb{C})$ then X has a non unique unitary decomposition $X = \sum_{i=1}^n \lambda_i U_i$. We then define the unitary norm as

$$\|X\|_U = \inf \sum_{i=1}^n |\lambda_i|. \quad (2.6)$$

Where the infimum runs over all decompositions $X = \sum_i \lambda_i U_i$ with the U_i 's unitary.

Carrying on our discussion, we continue with the following lemma.

Lemma 2.3. For all $X \in B(\mathcal{H})$, we have that $\|X\| = \|X\|_U$.

Proof. Suppose that $\|X\| = 1$, we can then employ the theorem to note that a convex combination of unitary operators yields X . This implies that for each $\varepsilon > 0$ $\left\| \frac{1}{2+\varepsilon} X \right\|_U \leq 1$. We then have that $\frac{1}{2} \|X\|_U \leq \|X\|$. Furthermore, let $X = \sum_{i=1}^n \lambda_i U_i$ for U_i unitary. Then we have by the triangle inequality that

$$\|X\| \leq \sum_{i=1}^n |\lambda_i| \|U_i\| = \sum_{i=1}^n |\lambda_i|. \quad (2.7)$$

Now taking the infimum over all representations we get the result $\|X\| \leq \|X\|_U$. We thus obtain $\frac{1}{2} \|X\|_U \leq \|X\| \leq \|X\|_U$. Therefore, the norms are equivalent. Applying the density of convex combinations of unitary operators in the unit sphere, we can generate a sequence of operators $(X_n)_{n=1}^\infty$ with $\|X_n\|_U = 1$ and converging to X . Hence, by this convergence we also know $\|X\|_U = 1$. We thus have in general that $\|X\| = \|X\|_U$, since we can write any operator X as $X = \|X\| \left(\frac{X}{\|X\|} \right)$. The operator $\frac{X}{\|X\|}$ has norm smaller or equal than one. ■

To make our lives more convenient we will use the following notation.

Notation 2.4. Given a set of operators on a Hilbert space \mathcal{H} denoted by M , we will write M_U to denote the unitary operators.

We now move on to the result commonly referred to as the Russo-Dye theorem.

Theorem 2.5 (Russo-Dye). For a linear map $\Phi : M_n(\mathbb{C}) \rightarrow M_n(\mathbb{C})$ we have that

$$\|\Phi\| = \sup_{U \in M_n(\mathbb{C})_U} \|\Phi(U)\|.$$

Furthermore, if Φ is unital then Φ is positive if and only if $\|\Phi\| = 1$.

Proof of the first part of the theorem. Let $X \in B(\mathcal{H})$ then X has a unitary decomposition given as $X = \sum_i \lambda_i U_i$ for U_i unitary for all i . Hence, $\|U_i\| = 1$ for all i . Then we have that

$$\begin{aligned} \|\Phi(X)\| &\leq \sum_i |\lambda_i| \sup_{U \in M_n(\mathbb{C})_U} \|\Phi(U)\| \\ &= \|X\|_U \sup_{U \in M_n(\mathbb{C})_U} \|\Phi(U)\| \\ &= \|X\| \sup_{U \in M_n(\mathbb{C})_U} \|\Phi(U)\|. \end{aligned}$$

In this equation we have applied the previous lemma to obtain the final equality. Dividing the norm of X to the other side and taking the supremum yields the required equality. ■

To prove the second part of the theorem we need to introduce a definition regarding a state on the bounded operators. It is important to note that this is different from the quantum state we defined before.

Definition 2.6. A state on $B(\mathcal{H})$ is a linear functional $\omega \in B(\mathcal{H})^*$ such that $\omega(X^*X) \geq 0$ for all $X \in B(\mathcal{H})$ i.e. ω is positive and we additionally require $\|\omega\| = 1$.

Notice that positivity for X^*X implies that ω is positive for all $X \geq 0$, by the fact that any element $X \geq 0$ has a decomposition as $X = A^*A$. Additionally, it should be noted that this is actually a more general definition of a quantum state, to see this let $\omega(X) = \langle \xi, X\xi \rangle$ for $\xi \in \mathcal{H}$ with $\|\xi\| = 1$ for some Hilbert space \mathcal{H} and $X \in B(\mathcal{H})$ then ω defines a state. Furthermore, by definition $\omega(X) = \langle X \rangle = \langle \xi, X\xi \rangle$ on the quantum state ξ . Hence, the functional state corresponds to the quantum state by the inner product. Additionally, for density matrices we have that $\langle X \rangle = \text{Tr}(\rho X)$, which can be seen by simple computation. Furthermore, we have that

$$\text{Tr}(\rho X) = \sum_{i=1}^n p_i \text{Tr}(\xi_i \xi_i^* X) = \sum_{i=1}^n p_i \text{Tr}(\xi_i^* X \xi_i) = \sum_{i=1}^n p_i \langle \xi_i, X \xi_i \rangle. \quad (2.8)$$

Hence, $\text{Tr}(\rho X)$ also defines a state. This shows the correspondence between quantum mechanical states of a system encoded in ρ and the general state definition.

To see that functional states actually help us prove the second part of the Russo-Dye theorem we require the following lemma which is adapted from Caspers [7] (Theorem 5.4).

Lemma 2.7. Let $\omega \in B(\mathcal{H})^*$. Then $\omega \geq 0$ if and only if for the sequence with $e_n = I$ for all $n \in \mathbb{N}$, we have $\|\omega\| = \lim_{n \rightarrow \infty} \omega(e_n)$.

Proof. In this entire proof we will again use the fact that we can re-scale the operator to assume $\|\omega\| = 1$.

For the forward implication, consider $\omega \geq 0$. By the fact that ω is positive, which makes $\omega(e_n)_{n=1}^{\infty}$ increasing, and bounded by 1, we can apply the monotone convergence theorem to conclude that the limit of $n \rightarrow \infty$ exists. Let $X \in B(\mathcal{H})$ a contraction, i.e. $\|X\| \leq 1$. Now we define an inner product on $B(\mathcal{H})$ by setting $\langle A, B \rangle = \omega(B^*A)$ for $A, B \in B(\mathcal{H})$. Notice that this results in a Cauchy-Schwarz inequality for the operator

$$|\omega(A^*B)|^2 \leq \omega(A^*A)\omega(B^*B). \quad (2.9)$$

Which yields the following

$$|\omega(Xe_n)|^2 \leq \omega(X^*X)\omega(e_n^2) \leq \|X\|^2\omega(e_n) \leq \omega(e_n). \quad (2.10)$$

In the last inequality we applied the fact that X is a contraction. If we take the limit in n we obtain $|\omega(X)|^2 \leq \lim_{n \rightarrow \infty} \omega(e_n)$. Since $\|\omega\| = 1$, we have $1 \leq \lim_{n \rightarrow \infty} \omega(e_n)$. Therefore, $\lim_{n \rightarrow \infty} \omega(e_n) = 1$.

For the backward implication, let $(e_n)_{n=1}^{\infty} = I$ with $\lim_{n \rightarrow \infty} \omega(e_n) = 1$. Then we will write $\omega(X) = \alpha + i\beta$ with $\alpha, \beta \in \mathbb{R}$ for $X \in B(\mathcal{H})$ with X a contraction and self-adjoint. Assume $\beta \leq 0$ (for $\beta > 0$ the proof goes similarly) and let $m \in \mathbb{N}$ then

$$\lim_{n \rightarrow \infty} \omega(X - ime_n) = \omega(X) - im = \alpha + i\beta - im. \quad (2.11)$$

Additionally, we can derive that

$$\begin{aligned}
\|\omega(X - ime_n)\|^2 &\leq \|\omega\|^2 \|X - ime_n\|^2 \\
&= \|X - ime_n\|^2 \\
&= \|(X + ime_n)(X - ime_n)\| \\
&= \|X^2 + m^2 e_n^2 - im[X, e_n]\| \\
&\leq 1 + m^2 + m\|[X, e_n]\|.
\end{aligned}$$

Where we used the triangle inequality and the fact that X is a contraction. Furthermore, $\lim_{n \rightarrow \infty} [X, e_n] = 0$ by definition of the approximate unit. Combining these results with 2.11 yields

$$\alpha^2 + \beta^2 - 2m\beta + m^2 = |\alpha + i\beta - im|^2 \leq 1 + m^2. \quad (2.12)$$

Therefore, $-2m\beta \leq 1 - \beta^2 - \alpha^2$, which cannot hold for large m unless $\beta = 0$. Thus for self-adjoint elements ω is real. Now let $X \in B(\mathcal{H})$ be a positive contraction. Then $\|e_n - X\| \leq 1$ by positivity of X , notice that $e_n - X$ is a self-adjoint element. Hence, $\omega(e_n - X) \leq 1$ and real. Furthermore,

$$1 - \omega(X) = \lim_{n \rightarrow \infty} \omega(e_n - X) \leq 1.$$

Thus $\omega(X) \geq 0$, which completes the proof. \blacksquare

We can now move on to the second statement, i.e. $\Phi(I) = I$ then Φ is positive if and only if $\|\Phi\| = 1$.

Proof of the second part of the Russo-Dye theorem. For the forward implication we apply the shorter and more efficient proof proposed by Bhatia [2] (pages 40-41). To this end, consider the following matrix for an arbitrary contraction operator $\|U\| \leq 1$, $U \in B(\mathcal{H})$

$$\hat{U} = \begin{pmatrix} U & -(I - UU^*)^{1/2} \\ (I - U^*U)^{1/2} & U^* \end{pmatrix}. \quad (2.13)$$

This is a unitary element in $M_2(B(\mathcal{H}))$. Furthermore, if we define Ψ to be the mapping that is the restriction to the top left hand corner, i.e. $\Psi(\hat{U}) = P\hat{U}P = U$, where P is the projection to the first coordinates. Then Ψ is positive and trivially unital. This can be seen as follows, assume $\hat{U} \geq 0$ then

$$(\xi_1, \xi_2)^* \begin{pmatrix} U & -(I - UU^*)^{1/2} \\ (I - U^*U)^{1/2} & U^* \end{pmatrix} (\xi_1, \xi_2) \geq 0. \quad (2.14)$$

In this equation $\xi_1, \xi_2 \in \mathcal{H}$, which yields after taking the inner product

$$\begin{aligned}
\langle \xi_1, U\xi_1 \rangle - \langle \xi_1, (I - UU^*)^{1/2} \xi_2 \rangle + \langle \xi_2, (I - U^*U)^{1/2} \xi_1 \rangle + \langle U\xi_2, \xi_2 \rangle &= \langle \xi_1, U\xi_1 \rangle + \langle \xi_2, U\xi_2 \rangle \\
&\geq 0.
\end{aligned}$$

Since this is true for every ξ_1, ξ_2 , we must have that $U \geq 0$. Hence, $\Psi \geq 0$. Because of the fact that this is a unitary element, it is also normal. Hence, we can apply the Kadison-Schwarz inequality on the map $\Phi \circ \Psi$, which is unital and positive. This yields

$$\begin{aligned}
(\Phi \circ \Psi(\hat{U}))(\Phi \circ \Psi(\hat{U}^*)) &\leq \Phi \circ \Psi(I), \\
\Phi(U)\Phi(U^*) &\leq I.
\end{aligned}$$

Which shows that $\|\Phi(U)\| \leq 1$ whenever U is a contraction, by taking the norm on both sides of the previous equation. Therefore, $\|\Phi\| = 1$.

For the backward implication let $\xi \in \mathcal{H}$ be a state in the quantum mechanical sense, i.e. ξ is a unit vector. Then $\omega(X) = \langle \Phi(X)\xi, \xi \rangle$ is a linear functional with norm $= \|\Phi\| = 1$ and value 1 at I . Hence, by the previous lemma, this is a state. Therefore, $X \geq 0$ forces $\omega(X) \geq 0$, which implies $\Phi(X) \geq 0$. Hence, Φ is positive. \blacksquare

2.2. COMPLETELY DISSIPATIVE OPERATORS

In this section we discuss the dissipative operator and show the equivalence of a generator being dissipative and its induced map obeying the Cauchy-Schwarz inequality. Furthermore, we will note a very important result regarding the domain of the dissipative operator, which determines the generator up to a Hamiltonian.

In this part we will use the identification of semi groups as made stated in 1.28 where for some generator L we set $\Phi_t = e^{tL}$. Furthermore, we assume that $\Phi(I) = I$, i.e. our semi group is unital. Additionally, for the extension to CP maps, we consider $L_n = L \otimes I_n$ with $\Phi_t^{(n)} = \Phi_t \otimes I_n = e^{tL_n}$, where we used the definition of the exponential to obtain the final equality.

2.2.1. EQUIVALENCE BETWEEN KADISON-SCHWARZ AND RUSSO-DYE

Using the previously mentioned assumptions we start the discussion on dissipative operators. We define the type of operators and prove the equivalence of generators being dissipative operators and the induced map obeying the Kadison-Schwarz inequality. This section is partially adapted from Lindblad [16].

To this end, take into consideration the Kadison-Schwarz inequality, which after taking the derivative with respect to t yields

$$\begin{aligned} \left. \frac{d}{dt} \right|_{t=0} (\Phi_t(X^*X) - \Phi_t(X^*)\Phi_t(X)) &\geq 0 \\ L_n e^{tL_n} X^* X - L_n e^{tL_n} X^* e^{tL_n} X - e^{tL_n} X^* L_n e^{tL_n} &\Big|_{t=0} \geq 0 \\ L_n(X^*X) - L_n(X^*)X - X^*L_n(X) &\geq 0. \end{aligned} \tag{2.15}$$

In this equation we used the fact that $\Phi_t^{(n)}(I) = I$. Furthermore, we define the following

Definition 2.8. If a bounded map $L : B(\mathcal{H}) \rightarrow B(\mathcal{H})$ satisfies $L(I) = 0$ and $L(X^*) = L(X)^*$ for all $X \in B(\mathcal{H})$ (L is a $*$ -map) and the function $D(L_n; X, X) \geq 0$ for all $X \in M_n(B(\mathcal{H}))$ and for all $n \in \mathbb{N}$. For $D(L; X, Y)$ the dissipation function defined as

$$D(L; X, Y) = L(X^*Y) - L(X^*)Y - X^*L(Y). \tag{2.16}$$

Then L is said to be completely dissipative, which we denote as $L \in \text{CD}(B(\mathcal{H}))$.

Additionally, note that in our case derived before $L \in \text{CD}(B(\mathcal{H}))$, since $\Phi_t(I) = I$ and $\Phi_t \in \text{CP}(B(\mathcal{H}))$ implies $L_n(I) = 0$ and $L_n(X^*) = L_n(X)^*$. This identification is actually more general, which is contained in the following proposition.

Proposition 2.9. Let $L : B(\mathcal{H}) \rightarrow B(\mathcal{H})$ be a bounded $*$ -map and let $\Phi_t = e^{tL}$. Then the following are equivalent:

- a) $\Phi_t(X^*X) \geq \Phi_t(X^*)\Phi_t(X)$ for all $X \in B(\mathcal{H})$ and $\Phi_t(I) = I$.
- b) $D(L; X, X) \geq 0$ for all $X \in B(\mathcal{H})$ and $L(I) = 0$.

As noted before the statement of the proposition, by the previous discussion we have already shown $a \implies b$. Hence, we are only left with $b \implies a$. To this end, note that Lumer and Phillips [17] proved the following identification

Lemma 2.10. A bounded operator L on $B(\mathcal{H})$ generates a semi-group of contraction operators if and only if $\Theta(L) \leq 0$ with

$$\Theta(L) = \lim_{t \rightarrow 0^+} \frac{\|I + tL\| - 1}{t}. \quad (2.17)$$

This is a similar definition to equation 1.31, however, it is less general since this only works for operators of the form e^{tL} with $\|e^{tL}\| \leq 1$. This theorem will be our main tool in proving the other implication.

Proof of proposition 2.9. Recall theorem 2.5 which implies $\|I + tL\| = \sup_{U \in B(\mathcal{H})} \|(I + tL)U\|$. By assumption we have that equation 2.15 yields

$$\begin{aligned} \|U + tL(U)\|^2 &\leq \|I + t(L(U^*)U + U^*L(U)) + t^2L(U^*)L(U)\|^2 \\ &\leq \|I + tL(I) + t^2L(U^*)L(U)\|^2 \\ &\leq \|I + t^2L(U^*)L(U)\|^2 \\ &\leq 1 + t^2\|L\|^2. \end{aligned}$$

Furthermore,

$$\sqrt{1 + t^2\|L\|^2} \leq 1 + t^2\|L\|^2.$$

Which implies that

$$\begin{aligned} \|I + tL\| &\leq 1 + t^2\|L\|^2 \\ \frac{\|I + tL\| - 1}{t} &\leq t\|L\|^2 \rightarrow 0 \text{ (in norm), } t \rightarrow 0^+. \end{aligned}$$

Hence, under the assumption we have that L generates a contractive semigroup by lemma 2.10. Notice that in this case we have that $\Phi_t(I) = I$ by the $L(I) = 0$ assumption. Moreover, since Φ_t is a contraction $\|\Phi_t\| \leq 1$, but by $\Phi_t(I) = I$ we have that $\|\Phi_t\| = 1$. Therefore, by the Russo-Dye theorem we have that $\Phi_t \geq 0$. This argument can be repeated for $L \in \text{CD}(B(\mathcal{H}))$ to obtain $\Phi_t^{(n)} \geq 0$, i.e. $\Phi_t \in \text{CP}(B(\mathcal{H}))$. We can now define the following function

$$S_\lambda = \lambda \int_0^\infty e^{-\lambda t} \Phi_t dt \quad \lambda > 0. \quad (2.18)$$

Setting $\Phi_t = e^{tL}$ yields that $S_\lambda = \lambda(\lambda - L)^{-1}$ and by positivity of Φ_t , this is a positive function. By applying the Russo-Dye theorem again, we see that $\|S_\lambda\| = 1$. Notice that choosing $\lambda = n/t$

for some $n \in \mathbb{N}$ gives

$$\begin{aligned} (S_{n/t})^n &= \left(\frac{n}{t} \left(\frac{n}{t} - L \right)^{-1} \right)^n \\ &= \left(1 - \frac{Lt}{n} \right)^{-n}. \end{aligned}$$

Sending $n \rightarrow \infty$ yields e^{tL} which is precisely what we wanted. However, we have not yet obtained the Cauchy-Schwarz inequality. To this end let $Y = (\lambda - L)^{-1}X$ for some $X \in B(\mathcal{H})$. Then we have

$$\begin{aligned} S_\lambda(X^*X) &\geq S_\lambda(\lambda^2 Y^*Y - \lambda(L(Y^*)Y - Y^*L(Y)) + L(Y^*)L(Y)) \\ &\geq S_\lambda(\lambda(\lambda - L)Y^*Y) \\ &= \lambda(\lambda - L)^{-1}\lambda(\lambda - L)Y^*Y \\ &= \lambda^2 Y^*Y \\ &= \lambda^2(\lambda - L)^{-1}X^*(\lambda - L)^{-1}X \\ &= S_\lambda(X^*)S_\lambda(X). \end{aligned}$$

Hence, we have obtained

$$S_\lambda(X^*)S_\lambda(X) \leq S_\lambda(X^*X). \quad (2.19)$$

Since this is true for all λ , by continuity and sending $n \rightarrow \infty$ it is also true for e^{tL} which completes the proof. \blacksquare

Applying this proposition to the extensions L_n and $\Phi_t^{(n)}$ yields the following corollary.

Corollary 2.11. Let $L : B(\mathcal{H}) \rightarrow B(\mathcal{H})$ be a bounded map $*$ -map and let $\Phi_t = e^{tL}$. Then $\Phi_t \in \text{CP}(B(\mathcal{H}))$ with Φ_t unital if and only if $L \in \text{CD}(B(\mathcal{H}))$. Furthermore, Φ_t is norm continuous if L is ultraweakly continuous.

2.2.2. DETERMINATION OF A CD-GENERATOR

In this subsection we consider the dissipation function of the a completely dissipative generator L . We do this in two parts. Firstly, we define the Haar measure. Secondly, we prove that $D(L)$ determines L up to Hamiltonian.

THE HAAR MEASURE

In this part we define the Haar measure and its properties. We begin with defining a topological group.

Definition 2.12. A topological space (A, τ) endowed with a group operation $\circ : A \times A \rightarrow A$ is a topological group if

1. Group multiplication $(g, h) \mapsto gh$ of $X \times X \rightarrow X$ is continuous
2. Group inversion $g \mapsto g^{-1}$ of $X \rightarrow X$ is continuous.

In the rest of this thesis we will assume a topological group to also be Hausdorff. Additionally, to illustrate this concept consider the following example

Example 2.1. The space $\mathbb{S}^1 = \{e^{i\theta} : 0 \leq \theta < 2\pi\}$ endowed with the regular e-power multiplication

$$\circ : \mathbb{S}^1 \times \mathbb{S}^1 \rightarrow \mathbb{S}^1, \quad (e^{it}, e^{is}) \mapsto e^{i(t+s)} \quad (2.20)$$

and the regular inversion

$$^{-1} : \mathbb{S}^1 \rightarrow \mathbb{S}^1, \quad e^{it} \mapsto e^{-it} \quad (2.21)$$

is a topological group.

To actually define the Haar measure, we also need to define the generalisation of the Lebesgue measure, called the Radon measure. The Radon measure is defined as

Definition 2.13. A Radon measure is a measure μ defined on a Hausdorff topological space, which has the following two properties:

1. μ is locally finite.
2. μ is inner regular.

The Radon measure is a measure, which respects and takes into account the topology of a topological space. The Hausdorffness is required to obey the first property. Namely

Definition 2.14. A measure $\mu : \Sigma \rightarrow \mathbb{R}$ for Σ some σ -algebra of a Hausdorff topological space (A, τ) is said to be locally finite if:

1. $\tau \subset \Sigma$.
2. For all $x \in A$, there exists an open neighborhood $U_x \in \tau$ such that $\mu(U_x) < \infty$.

Additionally, we need to define what inner regular means. This property has to do with approximating measures of arbitrary sets in the σ -algebra with compact sets. It is defined as

Definition 2.15. Consider the same setup as in the previous definition. Then a measure $\mu : \Sigma \rightarrow \mathbb{R}$ is said to inner regular if:

1. $\tau \subset \Sigma$.
2. $\forall X \in \Sigma$ we have that

$$\mu(X) = \sup \{ \mu(K) : K \text{ is compact, } K \subset X \}. \quad (2.22)$$

As an example, the Lebesgue measure is a Radon measure. Since we have now defined the Radon measure, we can move on to the Haar measure, which Folland [9] (pages 36-40) defined as

Definition 2.16. Let G be a locally compact topological group. Let Σ be the σ -algebra of subsets of G , where we require that it contains the Borel subsets. A Radon measure $\mu : \Sigma \rightarrow \mathbb{R}$ is called a left invariant Haar measure on G is $\mu(gE) = \mu(E)$ for every Borel set $E \subset G$ and every $g \in G$.

This is a clear definition regarding the topological group G . However, to construct integrals, we will need more formalism. To this end consider the following set of continuous functions on a locally compact group G

$$C_c(G) = \{f : f^{-1}(\{0\}^c) \text{ is compact}\}. \quad (2.23)$$

This set is called the space of compactly supported continuous functions, since the set where f is non zero has to be compact. Furthermore, we have that in Folland [9] the following theorem is proved.

Theorem 2.17. Every locally compact group G possesses a left invariant Haar integral defined on $C_c(G)$. Where the Haar integral is given with respect to a Haar measure μ by

$$\int_G L_g f d\mu = \int_G f d\mu. \quad (2.24)$$

In the equation L_g is defined to be operating as $L_g f(x) = f(g^{-1}x)$, where $g \in G$. For right invariance we would simply write the same integral with $R_g f(x) = f(xg)$.

We will not prove this fact, but it is important to note, because it allows us to claim that this integral exist, whenever we have a locally compact group. This will be used later in the proof of the Lindblad equation.

DETERMINING A GENERATOR FROM THE DISSIPATION FUNCTION

In this section we consider the dissipation function $D(L; X, Y)$ of a generator $L \in \text{CD}(B(\mathcal{H}))$. We prove the following theorem proposed by Lindblad [16].

Theorem 2.18. The dissipation function $D(L; X, Y)$ for $L \in \text{CD}(B(\mathcal{H}))$ determines L up to Hamiltonian.

This theorem is fundamental in giving physical significance to the concepts introduced thus far. However, to prove it, we will first need to introduce the definition of a derivation and prove an auxiliary lemma proved by Nayak [20].

Definition 2.19. A derivation $\mathcal{D} : B(\mathcal{H}) \rightarrow B(\mathcal{H})$ is a linear transformation that obeys the Leibniz rule, i.e.

$$\mathcal{D}(AB) = A\mathcal{D}(B) + \mathcal{D}(A)B, \quad \text{for all } A, B \in B(\mathcal{H}). \quad (2.25)$$

The simplest example of a derivation is the derivative on the continuous space of functions, which obeys the product rule. The product rule in this case is identical to the Leibniz rule, hence by linearity of the derivative this is a derivation. The definition leads to the following lemma often called the derivation theorem.

Lemma 2.20 (Derivation theorem). Let \mathcal{D} be a derivation on $M_n(\mathbb{C})$. Then there exists a matrix $Z \in M_n(\mathbb{C})$ such that $\mathcal{D}(A) = [Z, A]$ for all $A \in M_n(\mathbb{C})$. Additionally, Z is unique up to translation with a scalar matrix. Letting $M_n(\mathbb{C})_U$ the compact group of unitary matrices with the left-invariant Haar measure on $M_n(\mathbb{C})_U$ denoted by dU . We have that Z is given by

$$Z = \alpha I + \int_{M_n(\mathbb{C})_U} \mathcal{D}(U)U^{-1}dU. \quad (2.26)$$

In this lemma we stated that $M_n(\mathbb{C})_U$ is a compact topological group. To see this let $M_n(\mathbb{C})_U$ be endowed with the regular matrix multiplication. Since this is polynomial in all the entries, we have that this multiplication is continuous in the norm topology. Furthermore, note that conjugate transposition is a continuous operation in the 2-norm ($\|\cdot\|_2$) and because all norms are equivalent on finite dimensional spaces, we have that conjugate transposition is also a norm continuous operation. Furthermore, we know that conjugate transposition is inversion for unitary matrices. Hence, this actually proves that $M_n(\mathbb{C})_U$ is a topological group. Additionally, compactness follows from the fact that the following functions are both continuous and both map to the identity matrix

$$\begin{aligned} f_1 : M_n(\mathbb{C}) &\rightarrow M_n(\mathbb{C}), & U &\mapsto U^*U = I \\ f_2 : M_n(\mathbb{C}) &\rightarrow M_n(\mathbb{C}), & U &\mapsto UU^* = I. \end{aligned}$$

Since these two functions are continuous and $M_n(\mathbb{C})_U$ can be written as

$$M_n(\mathbb{C})_U = f_1^{-1}(\{I\}) \cap f_2^{-1}(\{I\}). \quad (2.27)$$

We have that $M_n(\mathbb{C})_U$ is a closed and bounded set of an Euclidean space, hence it is compact. Here, the boundedness stems from the fact that $\|U\| = 1$ for all unitary matrices. Thus we have that $M_n(\mathbb{C})_U$ is a compact topological group. We now move on to the proof of the lemma provided by Nayak [20].

Proof of lemma 2.20. Define the following function

$$\psi_U(X) := UXU^{-1} + \mathcal{D}(U)U^{-1}, \quad \text{for } U \in M_n(\mathbb{C})_U. \quad (2.28)$$

We can then study the composition, hence let $U, V \in M_n(\mathbb{C})_U$ and $X \in M_n(\mathbb{C})$ then

$$\begin{aligned} \psi_V \circ \psi_U(X) &= V\psi_U(X)V^{-1} + \mathcal{D}(V)V^{-1} \\ &= V(UXU^{-1} + \mathcal{D}(U)U^{-1})V^{-1} + \mathcal{D}(V)V^{-1} \\ &= (VU)X(VU)^{-1} + (V\mathcal{D}(U) + \mathcal{D}(V)U)(VU)^{-1} \\ &= (VU)X(VU)^{-1} + (\mathcal{D}(VU))(VU)^{-1} \\ &= \psi_{VU}(X). \end{aligned}$$

In the second to last equality we used the Leibniz rule to derive the result. Thus our composition yields that for any $U, V \in M_n(\mathbb{C})_U$ we have that $\psi_U \circ \psi_V = \psi_{UV}$. Note that for any matrix X this function is a continuous function on the compact group, hence $\psi_U(X) \in C_c(G)$ for some fixed X . This allows us to define

$$Z := \int_{M_n(\mathbb{C})_U} \psi_U(X) dU. \quad \text{for some fixed } X \in M_n(\mathbb{C}). \quad (2.29)$$

Now let $V \in M_n(\mathbb{C})_U$ then we have by linearity that

$$\begin{aligned} \psi_V(Z) &= \psi_V \left(\int_{M_n(\mathbb{C})_U} \psi_U(X) dU \right) \\ &= \int_{M_n(\mathbb{C})_U} \psi_V \circ \psi_U(X) dU \\ &= \int_{M_n(\mathbb{C})_U} \psi_{VU}(X) dU. \end{aligned}$$

But the Haar measure was defined to be left invariant, which yields

$$\begin{aligned}
\int_{M_n(\mathbb{C})_U} \psi_{VU}(X) dU &= \int_{M_n(\mathbb{C})_U} L_V \psi_{VU}(X) dU \\
&= \int_{M_n(\mathbb{C})_U} (V(V^{-1}U))X(V(V^{-1}U))^{-1} + (\mathcal{D}(V(V^{-1}U)))(V(V^{-1}U))^{-1} dU \\
&= \int_{M_n(\mathbb{C})_U} \psi_U(X) dU \\
&= Z.
\end{aligned}$$

Hence, for all $U \in M_n(\mathbb{C})_U$ we have that $\psi_U(Z) = Z$. We then obtain that $UZU^{-1} + \mathcal{D}(U)U^{-1} = Z \iff UZ + \mathcal{D}(U) = ZU$, but this means that $\mathcal{D}(U) = [Z, U]$. As mentioned before any operator has a decomposition into unitary operators, since derivations are linear, we have that $\mathcal{D}(A) = [Z, A]$ for any $A \in M_n(\mathbb{C})$. Additionally, if both Z_1 and Z_2 obey the equation for \mathcal{D} , i.e. $[Z_1, A] = [Z_2, A]$. Then this implies that $[Z_1 - Z_2, A] = 0$. Which means that $Z_1 = \alpha I + Z_2$ for some $\alpha \in \mathbb{C}$. Hence, we are done. \blacksquare

Using this lemma, we can prove theorem 2.18.

Proof of theorem 2.18. If $L \in \text{CD}(B(\mathcal{H}))$ then $D(L; X, Y) \geq 0$ for all $X, Y \in B(\mathcal{H})$. Let us first consider the case $D(L; X, Y) = 0$. Then L is a derivation and we can immediately apply the previous lemma to conclude that $L(X) = [Z, X]$, where Z is given as in equation 2.26. Additionally, we know that L is a $*$ -map. Hence, $L(X)^* = L(X^*)$. This implies

$$L(X)^* = (ZX)^* - (XZ)^* = X^*Z^* - Z^*X^* = L(X^*) = ZX^* - X^*Z. \quad (2.30)$$

Hence, $Z = iH$ for H self-adjoint. Given this fact $\Phi_t(X) = e^{tL}(X) = e^{iHt}Xe^{-iHt}$. Which is precisely the time evolution of operators considered in the Heisenberg picture. Conversely, if L generates a semi group of CP maps, then both L and $-L$ have $D(L; X, X) \geq 0$ and $D(-L; X, X) \geq 0$. Hence, $D(L, X, X) = 0$, thus $L = i[H, X]$. In the case where $D(L; X, Y) \neq 0$, we thus have a lack of reversibility. Hence, no Hamiltonian equivalence. \blacksquare

3

THE LINDBLAD MASTER EQUATION

During this chapter the Lindblad master equation is derived using the previously built formalism. This derivation yields a general form for the generators of UCP maps. Additionally, a derivation from the microscopical point of view is discussed. Both these derivations yield the Lindblad master equation, which describes the evolution of a system interacting with a heat bath. This equation is of utmost importance in studying the physics of these evolutions.

3.1. THE LINDBLAD EQUATION FROM THE MATHEMATICAL SIDE

In this section we derive the Lindblad master equation from the mathematical principles we have developed so far in addition to the concept of hyperfiniteness, which will be discussed in the first part of this section, whilst the second part is used to derive the master equation.

3.1.1. HYPERFINITENESS

During this part we discuss the concept of hyperfiniteness and its use based on the discussion that the unitary elements of the finite $M_n(\mathbb{C})$ form a compact topological group.

In the previous section we have defined the Haar measure, which is useful due to it being left invariant. However, to use the Haar measure we require a compact topological group. The topological group we want to study is that of the unitary operators in $B(\mathcal{H})$. We begin with proving that the unitary operators actually form a topological group.

Proposition 3.1. The unitary operators $B(\mathcal{H})_U$ form a topological group.

This can immediately be seen in the case of finite dimensional operators, in which case we can simply use the identification $M_n(\mathbb{C}) \simeq B(\mathcal{H})$ and use the proof for $M_n(\mathbb{C})_U$ given in the proof of lemma 2.20. However, it can more generally be proven in the SOT, which does not require that assumption.

Proof. We start off with the composition. To this end let $\varepsilon > 0$ and let $x \in \mathcal{H}$. Additionally, we consider $(U, V) \mapsto UV$. Then using equation 1.26 we define an open set O around UV as

$$O(UV, x, \varepsilon) = \{A \in B(\mathcal{H})_U : \|(UV - A)x\| < \varepsilon\}. \quad (3.1)$$

Now set $W((U, V), x, \varepsilon) = \{(B, C) \in B(\mathcal{H})_U : \|(U - B)Cx\| < \frac{\varepsilon}{2}, \|(V - C)x\| < \frac{\varepsilon}{2}\}$. Then

$$\begin{aligned} \|(UV - BC)x\| &\leq \|(UV - UC)x\| + \|(UC - BC)x\| \\ &= \|U(V - C)x\| + \|(U - B)Cx\| \\ &= \|(V - C)x\| + \|(U - B)Cx\| \\ &< \frac{\varepsilon}{2} + \frac{\varepsilon}{2} = \varepsilon. \end{aligned}$$

Hence, we have found an open set in the pre-image, thus composition is continuous. To prove continuity of the inverse, consider the following set

$$O(U^*, x, \varepsilon) = \{A^* \in B(\mathcal{H})_U : \|(U^* - A^*)x\| < \varepsilon\}. \quad (3.2)$$

Define $W(U, x, \varepsilon) = \{B \in B(\mathcal{H})_U : \|(U - B)U^*x\| < \varepsilon\}$. Then for $A \in W(U, x\varepsilon)$ and setting $y = U^*x$ we have

$$\|(U^* - A^*)x\| = \|y - A^*Uy\| = \|Ay - Uy\| < \varepsilon.$$

Hence, the inverse is also continuous. Therefore, we can conclude that $B(\mathcal{H})_U$ is a topological group. ■

We now have obtained two approaches, which both show that $B(\mathcal{H})_U$ is a topological group. However, we still require that it is compact to be able to use the Haar measure. To show this we require the notion of hyperfiniteness, which will allow us to construct $B(\mathcal{H})$ out of finite sets. The definition of hyperfiniteness requires the weak*-topology and is defined by Sakai [23] (page 204) as

Definition 3.2. Let \mathcal{M} be the dual of a Banach space. Then if \mathcal{M} is a Banach algebra with an involution $*$ and $\|X\|^2 = \|X^*X\|$ for $X \in \mathcal{M}$ is called a hyperfinite factor if there exists an increasing sequence of type $I_{n(p)}$ subfactors $\{\mathcal{M}_p\}$ with $n(p) < \infty$ such that the weak* closure of $\bigcup_{p=1}^{\infty} \mathcal{M}_p$ is \mathcal{M} .

In this definition we have an increasing sequence, which implies that $\mathcal{M}_p \subset \mathcal{M}_{p+1}$. Furthermore, the type $I_{n(p)}$ subfactor is defined by Topping [25] (page 81) in the following way.

Definition 3.3. A type $I_{n(p)}$ subfactor \mathcal{M}_p is isomorphic to $M_{n(p)}(\mathbb{C})$ and $I \in \mathcal{M}_p$. Here I is the identity operator.

This definition is convenient, because if a space of operators is a hyperfinite factor, we can split it up into finite pieces $\{\mathcal{M}_p\}$. These finite pieces all contain unitary elements, which form a closed and bounded set, hence by Bolzano-Weierstrass we immediately have that this is a compact set for every p . Since we already proved that the unitary elements formed a topological group, we now have a compact topological group. This fact allows us to define an invariant mean \mathcal{N}_p defined by the Haar measure for every p on the unitary elements of \mathcal{M}_p .

3.1.2. DERIVATION OF THE MASTER EQUATION

This part we derive the Lindblad equation by stating and proving the two most important propositions of Lindblads paper.

To obtain the master equation we require the mean \mathcal{N}_p as discussed above, this allows to propose the following proposition from Lindblad [16].

Proposition 3.4. Suppose $L \in \text{CD}(B(\mathcal{H}))$, with L weak* continuous. Then there is a $\Psi \in \text{CP}(B(\mathcal{H}))$ and a self adjoint $H \in B(\mathcal{H})$ such that for all $X \in B(\mathcal{H})$ we have

$$L(X) = \Psi(X) - \frac{1}{2}\{\Psi(I), X\} + i[H, X]. \quad (3.3)$$

In this equation $\{A, B\} = AB + BA$, i.e. the anticommutator.

Proof. By Topping [25] (pages 91-92) we know that $B(\mathcal{H})$ is actually a hyperfinite factor. Hence, we can define an invariant mean \mathcal{N}_p as discussed before. Additionally, we define $K_p \in B(\mathcal{H})$ as $K_p = \mathcal{N}_p(L(U^*)U)$, which immediately implies that $\|K_p\| \leq \|L\|$. We can now use the left invariance for any unitary $V \in \mathcal{M}_p$ to obtain

$$\mathcal{N}_p(L(VU^*)U) = \mathcal{N}_p(R_V[L(VU^*)U]) = \mathcal{N}_p(L(V(UV)^*)UV) = \mathcal{N}_p(L(U^*)UV) = K_p V. \quad (3.4)$$

Recall that \mathcal{N}_p is an invariant integral over the unitary elements of \mathcal{M}_p , i.e. independent of V . This implies that we can pull V out of the integral to derive the last equality. Thus invoking the fact that any operator can be written as a finite linear combination of unitaries, we deduce that $\mathcal{N}_p(L(XU^*)U) = K_p X$. Using this fact we can consider the dissipation function (equation 2.16) of L for any $X, Y \in \mathcal{M}_p$ as follows

$$\begin{aligned} \mathcal{N}_p(D(L; UX, UY)) &= \mathcal{N}_p(L((UX)^*UY) - L((UX)^*)UY - (UX)^*L(UY)) \\ &= L(X^*Y) - \mathcal{N}_p(L(X^*U)U)Y - X^*\mathcal{N}_p(U^*L(UY)) \\ &= L(X^*Y) - K_p X^*Y - X^*YK_p^*. \end{aligned}$$

Where we assumed that our Haar integral has unit volume for the unitary elements in \mathcal{M}_p , which can be done by rescaling. We define $\Psi_p : B(\mathcal{H}) \rightarrow B(\mathcal{H})$ by

$$\Psi_p(X) = L(X) - K_p X - X K_p^*. \quad (3.5)$$

Note that because L was picked in $\text{CD}(B(\mathcal{H}))$ we have that for every $X \in \mathcal{M}_p$ $\Psi_p(X^*X) = \mathcal{N}_p(D(L; UX, UX)) \geq 0$. Due to the fact that the dissipation function is non-negative and the integral of a non-negative function is again non-negative. Thus we have that $\Psi_p \geq 0$ on \mathcal{M}_p , since $X^*X \geq 0$ for all $X \in B(\mathcal{H})$. Applying the same argument to $M_n(\mathcal{M}_p)$ we find $\mathcal{N}_{pn}(L_n(U^*)U) = K_p \otimes I_n$, where \mathcal{N}_{pn} is the invariant mean on the unitary elements in $M_n(\mathcal{M}_p)$, which implies that $\Psi_p|_{\mathcal{M}_p} \in \text{CP}(\mathcal{M}_p, B(\mathcal{H}))$. Hence, Ψ_p defined in this way is completely positive when restricted to \mathcal{M}_p for each p . We can now generalise to obtain a Ψ on the entire space $B(\mathcal{H})$.

Let $\Psi_K = L(X) - KX - XK^*$ and define the following set

$$\Gamma_p = \{K \in B(\mathcal{H}) : \Psi|_{\mathcal{M}_p} \in \text{CP}(\mathcal{M}_p, B(\mathcal{H})), \|K\| \leq \|L\|\}. \quad (3.6)$$

Γ_p is precisely those K that yield a function similar to equation 3.5. The only part that remains is proving that there is at least one element K for which we can define Ψ_K such that it CP on the entire space. To this end, note that $K_p \in \Gamma_p$, i.e. $\Gamma_p \neq \emptyset$ for all p . Furthermore, due to the fact that we either increase or keep the amount of unitaries the same when comparing p and $p+1$. Every K that makes $\Psi_K|_{\mathcal{M}_{p+1}}$ CP must also make $\Psi_K|_{\mathcal{M}_p}$ CP. Hence, $\Gamma_{p+1} \subset \Gamma_p$. Furthermore, Γ_p is weakly closed. To see this assume that $(K_n)_{n=1}^\infty \subset \Gamma_p$ with $K_n \rightarrow K$ in the

WOT. Then we need to prove that $K \in \Gamma_p$. Firstly, note that if $\Phi_n \geq 0$ and $\Phi_n \rightarrow \Phi$ in the WOT, then $\Phi \geq 0$. This can be seen as follows, convergence in the WOT is given by

$$\langle \Phi_n \xi, \xi \rangle \rightarrow \langle \Phi \xi, \xi \rangle \quad \forall \xi \in \mathcal{H}. \quad (3.7)$$

Since convergence in the WOT holds for any pair $\xi, \eta \in \mathcal{H}$, it must definitely hold for $\xi, \xi \in \mathcal{H}$. Thus since $\langle \Phi_n \xi, \xi \rangle \geq 0$ we must have $\langle \Phi \xi, \xi \rangle \geq 0$. Apply this result to the fact that $K_n \rightarrow K$ weakly, which means that $\Psi_{K_n} \rightarrow \Psi_K$ weakly. Therefore, by using the same argument as before with L_n and $M_n(\mathcal{M}_p)$ we obtain that Ψ_K is CP on \mathcal{M}_p . Secondly, let $x \in \mathcal{H}$ a unit vector then

$$|\langle Kx, x \rangle| = \lim_{n \rightarrow \infty} |\langle K_n x, x \rangle| \leq \liminf_{n \rightarrow \infty} \|K_n\| \leq \|L\|. \quad (3.8)$$

Which after taking the supremum over all unit vectors x yields $\|K\| \leq \liminf_{n \rightarrow \infty} \|K_n\| \leq \|L\|$. Therefore, Γ_p is weakly closed for all p .

Furthermore, by the Banach-Alaoglu theorem the unit ball in $B(\mathcal{H})$ is weak* compact. Additionally, the weak*-topology and the weak topology coincide on the unit ball (for details see [19] theorem 4.2.4. and theorem 4.2.7), thus Γ_p is weakly-compact. Hence, $\Gamma = \bigcap_{p=1}^{\infty} \Gamma_p \neq \emptyset$. Thus, choose a $K \in \Gamma$. Then $\Psi = \Psi_K$ is CP on $\bigcup_{p=1}^{\infty} \mathcal{M}_p$. As L is weak* continuous we can now conclude that Ψ is CP on the weak*-closure of $\bigcup_{p=1}^{\infty} \mathcal{M}_p$. This follows from the fact that we can approximate any positive element $X \in \overline{\bigcup_{p=1}^{\infty} \mathcal{M}_p}$ in the weak*-topology with a positive sequence $X_n \in \bigcup_{p=1}^{\infty} \mathcal{M}_p$ (this fact is mainly a result from the Kaplansky theorem which is theorem 4.3.3. in Murphy [19]), which by weak* continuity of L implies, using the previous reasoning, that $L(X) \geq 0$ and thus Ψ is CP on the closure. Furthermore, note that $\Psi(I) = -K - K^*$. Then set $H = \frac{i}{2}(K^* - K)$. It follows that

$$\begin{aligned} L(X) &= \Psi(X) + KX + XK^* \\ &= \Psi(X) + \frac{1}{2}((K + K^*)X + (K - K^*)X) + \frac{1}{2}(X(K + K^*) + X(K^* - K)) \\ &= \Psi(X) + \frac{1}{2}((K + K^*)X + X(K + K^*)) + \frac{1}{2}((-K^* + K)X - X(-K^* + K)) \\ &= \Psi(X) - \frac{1}{2}((-K - K^*)X + X(-K - K^*)) + \frac{i}{2}(i(K^* - K)X - Xi(K^* - K)) \\ &= \Psi(X) - \frac{1}{2}(\Psi(I)X + X\Psi(I)) + i(HX - XH) \\ &= \Psi(X) - \frac{1}{2}\{\Psi(I), X\} + i[H, X] \end{aligned}$$

as required. ■

This is a powerful proposition, because it gives a general form for completely dissipative generators. However, we are not done yet, since we also want to go in the other direction. Suppose we have a Ψ which is CP and a self-adjoint $H \in B(\mathcal{H})$, does this yield a CD generator? It turns out that the answer to this question is actually yes, as captured in the following proposition.

Proposition 3.5. Let $\Psi \in \text{CP}(B(\mathcal{H}))$ and $H \in B(\mathcal{H})$ self-adjoint. Then L written as

$$L(X) = \Psi(X) - \frac{1}{2}\{\Psi(I), X\} + i[H, X] \quad (3.9)$$

has $L \in \text{CD}(B(\mathcal{H}))$.

Proof. To obtain the result, we utilise the Stinespring dilation as given in theorem 1.12, which states that if $\Psi \in \text{CP}(B(\mathcal{H}))$ we can write $\Psi(X) = V^* \pi(X) V$, for some $*$ -homomorphism π . Furthermore, we have that $L(I) = \Psi(I) - \frac{1}{2}\{\Psi(I), I\} + i[H, I] = 0$ and

$$L(X^*) = \Psi(X^*) - \frac{1}{2}\{\Psi(I), X^*\} + i[H, X^*] = \Psi(X)^* - \frac{1}{2}\{\Psi(I)^*, X\}^* + i[H^*, X]^* = L(X)^*. \quad (3.10)$$

Furthermore,

$$\begin{aligned} D(L; X, X) &= L(X^* X) - L(X^*) X - X^* L(X) \\ &= \Psi(X^* X) - \frac{1}{2}\{\Psi(I), X^* X\} + i[H, X^* X] - \Psi(X^*) X + \frac{1}{2}\{\Psi(I), X^*\} X - i[H, X^*] X \\ &\quad - X^* \Psi(X) + \frac{X^*}{2}\{\Psi(I), X\} - iX^*[H, X] \\ &= \Psi(X^* X) - \Psi(X^*) X - X^* \Psi(X) \\ &\quad - \frac{1}{2}[\Psi(I) X^* X + X^* X \Psi(I) - \Psi(I) X^* X - X^* \Psi(I) X - X^* \Psi(I) X - X^* X \Psi(I)] \\ &\quad + i[HX^* X - X^* XH - HX^* X + X^* HX + X^* XH - X^* HX] \\ &= \Psi(X^* X) - \Psi(X^*) X - X^* \Psi(X) + X^* \Psi(I) X. \end{aligned}$$

Additionally, for the Stinespring dilation we can choose $\pi(I) = I$ which yields

$$\begin{aligned} \Psi(X^* X) - \Psi(X^*) X - X^* \Psi(X) + X^* \Psi(I) X &= V^* \pi(X^* X) V - V^* \pi(X^*) V X - X^* V^* \pi(X) V + X^* V^* V X \\ &= V^* \pi(X^*) \pi(X) V - V^* \pi(X^*) V X - X^* V^* \pi(X) V + X^* V^* V X \\ &= (V^* \pi(X^*) - X^* V^*) (\pi(X) V - V X) \\ &= (\pi(X) V - V X)^* (\pi(X) V - V X) \geq 0, \end{aligned}$$

which completes the proof. ■

Notice that for the general form of L given in equation 3.3 we can apply the Choi-Kraus decomposition to obtain

$$L(X) = \sum_{i=1}^n (V_i^* X V_i - \frac{1}{2}\{V_i^* V_i, X\}) + i[H, X]. \quad (3.11)$$

This is the general form for the Lindblad master equation and it allows us to state the following theorem and main result from Lindblad [16].

Theorem 3.6. $L \in \text{CD}(\mathcal{H})$, with L weak $*$ continuous if and only if it is of the form

$$L(X) = \sum_{i=1}^n \left(V_i^* X V_i - \frac{1}{2}\{V_i^* V_i, X\} \right) + i[H, X], \quad (3.12)$$

where $V_i \in B(\mathcal{H})$, $\sum_i V_i^* V_i \in B(\mathcal{H})$ and $H \in B(\mathcal{H})$ is self-adjoint.

This theorem states the master equation in the Heisenberg picture. For the Schrödinger picture we can simply find the dual by letting ρ a density operator, then

$$\begin{aligned} \text{Tr} \left(\left[\sum_{i=1}^n (V_i^* X V_i - \frac{1}{2} \{V_i^* V_i, X\}) + i[H, X] \right] \rho \right) &= \sum_{i=1}^n \text{Tr}((V_i^* X V_i) \rho) - \frac{1}{2} \text{Tr}(\{V_i^* V_i, X\} \rho) + \text{Tr}(i[H, X] \rho) \\ &= \sum_{i=1}^n \text{Tr}(X V_i \rho V_i^*) - \frac{1}{2} \text{Tr}(X \rho V_i^* V_i + X V_i^* V_i \rho) \\ &\quad + \text{Tr}(i X \rho H - i X H \rho) \\ &= \text{Tr} \left(X \left[\sum_{i=1}^n V_i \rho V_i^* - \frac{1}{2} (\rho V_i^* V_i + X V_i^* V_i \rho) - i[H, \rho] \right] \right). \end{aligned}$$

Which yields that the general form for the Schrödinger picture Lindblad equation is given by

$$\begin{aligned} L^*(\rho) &= \frac{1}{2} \left(\sum_{i=1}^n 2V_i \rho V_i^* - \rho V_i^* V_i - V_i^* V_i \rho \right) - i[H, \rho] \\ &= \frac{1}{2} \left(\sum_{i=1}^n [V_i \rho, V_i^*] + [V_i, \rho V_i^*] \right) - i[H, \rho]. \end{aligned} \quad (3.13)$$

Equation 3.13 is the most general form for the Lindblad equation in the Schrödinger picture. Both equation 3.13 and equation 3.11 lets us describe the generators of dynamical semigroups explicitly. The physical significance of which is discussed in the next part.

3.1.3. PHYSICAL INTERPRETATION

In equation 3.11 we have found a general form for the generators of semigroups. However, what is the physical significance of this form? Why is it useful? These two questions will be answered during this part by considering a system in connection with a heat bath and deriving the evolutionary dynamics of the system.

Consider a system S in connection to a heat bath R , we can describe the entire system with a density operator $\rho_T = \sigma \otimes \rho$. Then for any operator $O(t)$ acting on the entire system, we can define its expectation value by

$$\langle O(t) \rangle = \text{Tr}(O(t) \rho_T) = \text{Tr}_S(\text{Tr}_R(O(t) \rho) \sigma) = \text{Tr}_S(\tilde{O}(t) \sigma). \quad (3.14)$$

Notice that $\tilde{O}(t)$ is now an operator on the system S , since the heat bath has been traced out. Furthermore, its expectation on system S can be calculated by multiplying with the density matrix of the system σ and tracing over the system. Hence, in the Heisenberg picture the development of S for a particular operator $X \in B(\mathcal{H}_S)$

$$X \mapsto \text{Tr}_R(U^*(X \otimes I)U\rho) = \Phi(X). \quad (3.15)$$

In this equation the $\otimes I$ represents the fact that the initial operator X acts on S and leaves the bath R alone. Furthermore, the U is a unitary operator which describes the time evolution according to a Hamiltonian as described in section 1.1.2. It turns out that this mapping is actually completely positive. We will prove this fact by using the partial trace in the Schrödinger picture.

Proposition 3.7. If $\rho_T = \sigma \otimes \rho$ is the density operator of a combined system consisting of system S with a heat bath R . Then the partial trace $\text{Tr}_R : \rho_T \rightarrow \sigma$ is a completely positive map.

Proof. To prove this let $(e_i)_i$ and $(f_j)_j$ be basis of \mathcal{H}_S and \mathcal{H}_R the Hilbert spaces describing the system S and bath R . Let $K_a = I_S \otimes f_a^*$, these will be the Kraus operators for the Choi-Kraus decomposition specified in the Choi-Kraus theorem 1.11. Now write $\rho_T = \sum_{i,j,k,h} \lambda_{ijkh} e_i e_j^* \otimes f_k f_h^*$, which has that $\text{Tr}_R(\rho_T) = \sum_{i,j,k,h} \lambda_{ijkh} e_i e_j^* \otimes f_k^*(f_k) f_h^*(f_h) = \sum_{i,j} \lambda_{ijja} e_i e_j^*$. Then we find that

$$\sum_a K_a \rho_T K_a^* = \sum_a I_S \otimes f_a^* \left(\sum_{i,j,k,h} \lambda_{ijkh} e_i e_j^* \otimes f_k f_h^* \right) I_S \otimes f_a = \sum_{i,j} \lambda_{ijja} e_i e_j^* = \text{Tr}_R(\rho_T). \quad (3.16)$$

Because the partial trace has a Kraus decomposition it is a CP map. ■

The fact that the partial trace is a CP map was first proved by Kraus. However, the proof above is a more eloquent version presented by Lidar [15] (pages 27-29). Notice that the mapping Φ defined in equation 3.15 is unital. Furthermore, Lindblad [16] also proved the converse, hence if we have such a CP operator it actually describes some sort of system evolution.

Proposition 3.8. If $\Phi \in \text{CP}(\mathcal{H}_1)$ and $\Phi(I) = I$ then there is an isometric operator V on $\mathcal{H}_1 \otimes \mathcal{H}_2$, where \mathcal{H}_2 is some Hilbert space such that for all ρ density operators on \mathcal{H}_2 we have

$$\Phi(X) = \text{Tr}_2(\rho V^*(X \otimes I_2)V). \quad (3.17)$$

Where I_2 is the identity on \mathcal{H}_1 .

Proof. We know that we can decompose Φ by the Choi-Kraus decomposition theorem 1.11 as

$$\Phi(X) = \sum_i V_i^* X V_i, \quad \sum_i V_i^* V_i = I. \quad (3.18)$$

Furthermore, suppose \mathcal{H}_2 is infinite dimensional. Then there are isometries in \mathcal{H}_2 such that $W_i^* W_j = \delta_{ij} I$, which leads us to define $V = \sum_i V_i \otimes W_i$. Then we have that

$$V^*(X \otimes I)V = \sum_i V_i^* X V_i \otimes W_i^* W_i = \Phi(X) \otimes I. \quad (3.19)$$

This leads to

$$\text{Tr}_2(V^*(X \otimes I)V) = \text{Tr}_2(\Phi(X) \otimes I) = \Phi(X). \quad (3.20)$$

Hence, we are done. ■

We have now found that CP maps describe the evolution of a system in connection to a heat bath. By applying the result that a generator L yields a one-parameter semigroup of operators e^{tL} we have immediately found the use of L . The semigroup describes the system at a time t and L generates this semigroup. This can also be seen by considering the evolution of the system in the Schrödinger picture, as captured in the following differential equation for a density operator ρ

$$\frac{d\rho}{dt} = L\rho. \quad (3.21)$$

The solution to this differential equation would be the one-parameter semigroup as discussed earlier. Notice that this is a little bit an abuse of notation, since previously L^* was the operator acting on the density matrix.

It is important to consider the different parts of the master equation. To this end consider the time evolution of a closed quantum system under Hamiltonian H . The evolution of the density operator ρ obeys the Von Neumann equation given as

$$\frac{d\rho}{dt} = -\frac{i}{\hbar} [H, \rho]. \quad (3.22)$$

This equation is easy to solve as

$$\rho(t) = e^{iHt/\hbar} \rho e^{-iHt/\hbar}. \quad (3.23)$$

Notice that this closed evolution is also contained in the Lindblad equation. However, the interesting physics is captured in the so-called dissipative part of the Lindblad equation

$$\frac{1}{2} \left(\sum_{i=1}^n [V_i \rho, V_i^*] + [V_i, \rho V_i^*] \right) = \sum_i V_i \rho V_i^* - \frac{1}{2} \rho V_i^* V_i - \frac{1}{2} V_i^* V_i \rho = \sum_i V_i \rho V_i - \frac{1}{2} \{V_i^* V_i, \rho\}. \quad (3.24)$$

The V_i , which were our Kraus operators, are often referred to as quantum jump operators or Lindblad operators. The $V_i^* \rho V_i$ describes the different jumps, whilst the other terms normalise the equation in the case no jumps occur.

3.2. MICROSCOPICAL DERIVATION

The mathematical derivation of the Lindblad equation is an airtight proof of the general form for generators of one-parameter semigroups. However, it is interesting to note that this equation can also be derived physically by making several assumptions that are physically valid, instead of abstract requirements. These assumptions should be such that we eventually derive the same equation. In this section we do exactly that: derive the master equation from physical principles and assumptions. To this end we will follow derivations by Manzano [18] and Brasil et al. [3].

3.2.1. THE REDFIELD EQUATION

In this section we are interested in studying the behaviour starting from a total system description given by the Von Neumann equation and obtaining the reduced dynamics of a system within this total system as described by the Redfield equation. To derive this equation we discuss the Markov and Born approximations which are required to obtain the result.

So far we have studied systems either in the Schrödinger or Heisenberg picture. However, to study interactions it is convenient to study the dynamics using the interaction picture, which is a hybrid of both Heisenberg and Schrödinger. In this picture the operators evolve with the separate Hamiltonians of the system and its environment, whilst the Schrödinger or Von Neumann equation contains the interaction Hamiltonian. To make this concrete consider the system S coupled to a heat bath R , which will be represented by Hilbert spaces \mathcal{H}_S and \mathcal{H}_R respectively. In this case the total system will be given by $\mathcal{H}_S \otimes \mathcal{H}_R$ with a total Hamiltonian defined by

$$H(t) = H_S \otimes I_R + I_S \otimes H_R + \alpha H_I. \quad (3.25)$$

In this equation we defined a coupling parameter α which determines the strength of the interaction described by the interaction Hamiltonian H_I . In the interaction picture we would now define a time dependent operator as

$$\hat{O}(t) = e^{i(H_S \otimes I_R + I_S \otimes H_R)t/\hbar} O e^{-i(H_S \otimes I_R + I_S \otimes H_R)t/\hbar} \quad (3.26)$$

where $O \in B(\mathcal{H}_S \otimes \mathcal{H}_R)$. Let $\rho_T = \sigma \otimes \rho$ describe the total density operator of the combined system then this step would reduce the Von Neumann equation as follows

$$\frac{d\rho_T}{dt}(t) = -\frac{i}{\hbar} [H(t), \rho_T(t)] \rightarrow \frac{d\hat{\rho}_T}{dt}(t) = -\frac{i\alpha}{\hbar} [\hat{H}_I(t), \hat{\rho}_T(t)]. \quad (3.27)$$

This equation is the starting point for the rest of the derivation. To this end consider that without loss of generality we can decompose $H_I = \sum_n S_n \otimes R_n$, where $S_n \in B(\mathcal{H}_S)$ and $R_n \in B(\mathcal{H}_R)$. Furthermore, we can assume that at $t = 0$ the total density operator can be written as $\rho_T(0) = \sigma(0) \otimes \rho(0)$. This can be achieved by not having the system interact with the heat bath beforehand. These two assumptions lead to the following lemma.

Lemma 3.9. Let $\rho(0)$ be the initial state of the heat bath. Then for operators R_n as given in the decomposition of H_I we can always redefine the total Hamiltonian $H(t)$ such that

$$\langle R_n \rangle = \text{Tr}(R_n \rho(0)) = 0. \quad (3.28)$$

Proof. Suppose that this is not already the case, then we can redefine the total Hamiltonian as

$$\begin{aligned} H(t) &= (H_S + \alpha \text{Tr}_R(H_I \rho(0))) \otimes I_R + I_S \otimes H_R + \alpha (H_I - \text{Tr}_R(H_I \rho(0))) \\ &= \left(H_S + \alpha \sum_n \langle R_n \rangle S_n \right) \otimes I_R + I_S \otimes H_R + \alpha \sum_n S_n \otimes (R_n - \langle R_n \rangle). \end{aligned}$$

Hence, the total Hamiltonian remains unchanged, but we have shifted parts. This implies the statement of the lemma, because $\langle R'_n \rangle = \langle R_n - \langle R_n \rangle \rangle = 0$. \blacksquare

It turns out that in a lot of physical systems $\text{Tr}_R(R_n \rho(0)) = 0$ automatically. However, if this is not the case we can apply the previous lemma. Furthermore, to actually derive the Lindblad equation we need two important assumptions or approximations: The Markov and Born approximation. These two assumptions not only play a crucial role in this derivation, but often show up in physics to simplify results. We start with the Born approximation which considers the correlation of the environment and the system. We know that due to the interaction Hamiltonian correlations will appear between the system and the reservoir. However, we can make the strong assumption that the correlation time and the relaxation time of the system are much smaller than the time scale of the system. We can only assume this in the weak coupling regime $\alpha \ll 1$, but even in this case it is still a strong assumption, which implies that $\rho_T(t) = \sigma(t) \otimes \rho(0)$. Hence, we have decoupled the system and the reservoir and assumed the reservoir is always in its initial state. This is the case if we for instance assume the reservoir to be a thermal state $\rho(0) = \frac{e^{-H_R \beta}}{\text{Tr}(e^{-H_R \beta})}$, where $\beta = 1/k_B T$. This is an assumption that is often used and we will assume it in the rest of the derivation as well. Apart from the Born approximation we must also consider the Markov assumption. This assumption concerns the fact that we

want our system to be memoryless, i.e. the evolution of a state can only depend on the state the system is currently in. Previous times are not allowed to be part of the equation. Using these two assumptions we can state the following lemma.

Lemma 3.10. Under the Born and Markovian assumption it is possible to describe the density operator of the system of interest ($\sigma(t)$) with the Redfield equation

$$\frac{d\sigma}{dt}(t) = -\frac{\alpha^2}{\hbar^2} \int_0^\infty \text{Tr}_R([\hat{H}_I(t_1), [\hat{H}_I(t-t_1), \hat{\sigma}(t) \otimes \hat{\rho}(0)]]) dt_1. \quad (3.29)$$

Proof. Starting from equation 3.27 we can integrate to obtain

$$\hat{\rho}_T(t) = \hat{\rho}_T(0) - \frac{i\alpha}{\hbar} \int_0^t [\hat{H}_I(t), \hat{\rho}_T(t_1)] dt_1. \quad (3.30)$$

Which after recombination with equation 3.27 yields

$$\frac{d\hat{\rho}_T}{dt}(t) = -\frac{i\alpha}{\hbar} [\hat{H}_I(t), \hat{\rho}_T(0)] - \frac{\alpha^2}{\hbar^2} \int_0^t [\hat{H}_I(t), [\hat{H}_I(t_1), \hat{\rho}_T(t_1)]] dt_1. \quad (3.31)$$

To obtain the dynamics of the density operator σ for system S, we must apply the partial trace, in turn tracing out the degrees of freedom of the heat bath. Furthermore, we can apply the Markov approximation to obtain the following

$$\begin{aligned} \text{Tr}_R\left(\frac{d\hat{\rho}_T}{dt}(t)\right) &= \frac{d\hat{\sigma}}{dt}(t) \\ &= -\frac{i\alpha}{\hbar} \text{Tr}_R([\hat{H}_I(t), \hat{\rho}_T(0)]) - \frac{\alpha^2}{\hbar^2} \int_0^t \text{Tr}_R([\hat{H}_I(t), [\hat{H}_I(t_1), \hat{\rho}_T(t_1)]]) dt_1. \end{aligned}$$

Let us for the moment focus on the first term, which evaluates to

$$\begin{aligned} \text{Tr}_R([\hat{H}_I(t), \hat{\rho}_T(0)]) &= \sum_n \text{Tr}_R([\hat{S}_n(t) \otimes \hat{R}_n(t), \hat{\sigma}(0) \otimes \hat{\rho}(0)]) \\ &= \sum_n \hat{S}_n(t) \hat{\sigma}(0) \text{Tr}_R(\hat{R}_n(t) \hat{\rho}(0)) - \hat{\sigma}(0) \hat{S}_n(t) \text{Tr}_R(\hat{\rho}(0) \hat{R}_n(t)) = 0. \end{aligned}$$

Where the last equality follows from the previous lemma and properties of the trace function. Furthermore, by applying the Born assumption we then obtain

$$\frac{d\hat{\sigma}}{dt}(t) = -\frac{\alpha^2}{\hbar^2} \int_0^t \text{Tr}_R([\hat{H}_I(t), [\hat{H}_I(t_1), \hat{\sigma}(t_1) \otimes \hat{\rho}(0)]]) dt_1. \quad (3.32)$$

Lastly, by applying the Markov assumption, we can replace t_1 in $\hat{\sigma}(t_1)$ with a t . Switching the variables $t_1 \mapsto t - t_1$ yields

$$\frac{d\hat{\sigma}}{dt}(t) = -\frac{\alpha^2}{\hbar^2} \int_0^t \text{Tr}_R([\hat{H}_I(t), [\hat{H}_I(t-t_1), \hat{\sigma}(t) \otimes \hat{\rho}(0)]]) dt_1. \quad (3.33)$$

Additionally, we can increase the upper limit of integration to infinity, without changing the outcome since we assume that the the system has no memory. Thus any effects different from $t_1 = t$ will decay quickly enough that increasing the limit has no effect which yields the Redfield equation.

$$\frac{d\hat{\sigma}}{dt}(t) = -\frac{\alpha^2}{\hbar^2} \int_0^\infty \text{Tr}_R([\hat{H}_I(t), [\hat{H}_I(t-t_1), \hat{\sigma}(t) \otimes \hat{\rho}(0)]]) dt_1. \quad (3.34)$$

■

3.2.2. THE EIGENBASIS OF $[H_S, \cdot]$

During this part we re-express the interaction Hamiltonian in the eigenbasis of $[H_S, \cdot]$ and use this to find a new expression of the Redfield equation.

Note that we are considering a finite dimensional system. Furthermore, by the self-adjointness of H_S there is a basis such that H_S is diagonal. Then by the spectral theorem the eigenvectors form a complete basis of $B(\mathcal{H}_S)$, i.e. there are operators $S_i(\omega) \in B(\mathcal{H}_S)$ such that

$$[H_S, S_i(\omega)] = -\omega S_i(\omega) \quad [H_S, S_i^*(\omega)] = \omega S_i^*(\omega). \quad (3.35)$$

In this equation the ω are the eigenvalues of $[H_S, \cdot]$. Hence, we can decompose the operators of the interaction Hamiltonian as $S_i = \sum_{\omega} S_i(\omega)$. Additionally, if in the infinite dimensional case the Hamiltonian can also be written as a diagonal operator, we can obtain the same result. Furthermore, we must expand the exponential operators in \hat{S}_n . Therefore, consider the following proposition.

Proposition 3.11. The interaction Hamiltonian $\hat{H}_I = \sum_n \hat{S}_n \otimes \hat{R}_n$ can be rewritten in the eigenbasis of H_S to

$$\hat{H}_I(t) = \sum_{n,\omega} e^{-i\omega t/\hbar} S_n(\omega) \otimes \hat{R}_n(t). \quad (3.36)$$

In this equation the ω are the eigenvalues of the operator $[H_S, \cdot]$. Additionally, we can also rewrite the interaction Hamiltonian as

$$\hat{H}_I(t) = \sum_{n,\omega} e^{i\omega t/\hbar} S_n^*(\omega) \otimes \hat{R}_n^*(t). \quad (3.37)$$

Proof. First note that the operator $\hat{S}_n(t) = \sum_{\omega} e^{itH_S/\hbar} S_n(\omega) e^{itH_S/\hbar}$. To derive the result of the proposition consider first the following

$$S_n H_S^k = ([S_n, H_S] + H_S S_n) H_S^{k-1} = (\omega I + H_S) (S_n H_S^{k-1}) = \dots = (\omega I + H_S)^k S_n. \quad (3.38)$$

Utilising this result yields

$$\begin{aligned} \hat{H}_I(t) &= \sum_n \hat{S}_n(t) \otimes \hat{R}_n(t) \\ &= \sum_{n,\omega} \sum_{k=0}^{\infty} \frac{(-it)^k}{k! \hbar^k} e^{itH_S/\hbar} S_n(\omega) H^k \otimes \hat{R}_n(t) \\ &= \sum_{n,\omega} \sum_{k=0}^{\infty} \frac{(-it)^k}{k! \hbar^k} e^{itH_S/\hbar} (\omega I + H_S)^k S_n(\omega) \otimes \hat{R}_n(t) \\ &= \sum_{n,\omega} e^{-i\omega t/\hbar} S_n(\omega) \otimes \hat{R}_n(t) \end{aligned}$$

■

This proposition is important because it allows us to rewrite the Redfield equation as shown in the next lemma.

Lemma 3.12. The Redfield equation can be rewritten to give the following

$$\frac{d\hat{\sigma}}{dt}(t) = \frac{\alpha^2}{\hbar^2} \sum_{\omega, \omega', k, l} \left(e^{i(\omega' - \omega)t/\hbar} \Gamma_{kl}(\omega) [S_l(\omega) \hat{\sigma}(t), S_k^*(\omega')] + e^{i(\omega' - \omega)t/\hbar} \Gamma_{lk}^*(\omega') [S_l(\omega), \hat{\sigma}(t) S_k^*(\omega')] \right). \quad (3.39)$$

Where $\Gamma_{kl}(\omega)$ is given as

$$\Gamma_{kl}(\omega) := \int_0^\infty e^{i\omega t_1/\hbar} \text{Tr}_R (\hat{R}_k^*(t) \hat{R}_l(t - t_1) \hat{\rho}(0)) dt_1. \quad (3.40)$$

Proof. First we expand the commutators in the Redfield equation to obtain

$$\begin{aligned} \frac{d\hat{\sigma}}{dt}(t) = & -\frac{\alpha^2}{\hbar^2} \text{Tr}_R \left[\int_0^\infty \hat{H}_I(t) \hat{H}_I(t - t_1) \hat{\sigma}(t) \otimes \hat{\rho}(0) dt_1 \right. \\ & - \int_0^\infty \hat{H}_I(t) \hat{\sigma}(t) \otimes \hat{\rho}(0) \hat{H}_I(t - t_1) dt_1 \\ & - \int_0^\infty \hat{H}_I(t - t_1) \hat{\sigma}(t) \otimes \hat{\rho}(0) \hat{H}_I(t) dt_1 \\ & \left. + \int_0^\infty \hat{\sigma}(t) \otimes \hat{\rho}(0) \hat{H}_I(t - t_1) \hat{H}_I(t) dt_1 \right]. \end{aligned}$$

Deriving the result relies on using the representations found for $\hat{H}_I(t)$ in the previous proposition, we will use the equation 3.36 for $\hat{H}_I(t - t_1)$ in term 1 and 3, whilst using equation 3.37 for term 2 and 4. Furthermore, we fill in equation 3.37 for $\hat{H}_I(t)$ in term 1 and 3, whilst using equation 3.36 for term 2 and 4. Which results in

$$\begin{aligned} \frac{d\hat{\sigma}}{dt}(t) = & -\frac{\alpha^2}{\hbar^2} \text{Tr}_R \left[\int_0^\infty \left(\sum_{k, \omega'} e^{i\omega' t/\hbar} S_k^*(\omega') \otimes \hat{R}_k^*(t) \right) \left(\sum_{l, \omega} e^{-i\omega(t-t_1)/\hbar} S_l(\omega) \otimes \hat{R}_l(t - t_1) \right) \hat{\sigma}(t) \otimes \hat{\rho}(0) dt_1 \right. \\ & - \int_0^\infty \left(\sum_{l, \omega} e^{-i\omega t/\hbar} S_l(\omega) \otimes \hat{R}_l(t) \right) \hat{\sigma}(t) \otimes \hat{\rho}(0) \left(\sum_{k, \omega'} e^{i\omega'(t-t_1)/\hbar} S_k^*(\omega') \otimes \hat{R}_k^*(t - t_1) \right) dt_1 \\ & - \int_0^\infty \left(\sum_{l, \omega} e^{-i\omega(t-t_1)/\hbar} S_l(\omega) \otimes \hat{R}_l(t - t_1) \right) \hat{\sigma}(t) \otimes \hat{\rho}(0) \left(\sum_{k, \omega'} e^{i\omega' t/\hbar} S_k^*(\omega') \otimes \hat{R}_k^*(t) \right) dt_1 \\ & \left. + \int_0^\infty \hat{\sigma}(t) \otimes \hat{\rho}(0) \left(\sum_{k, \omega'} e^{i\omega'(t-t_1)/\hbar} S_k^*(\omega') \otimes \hat{R}_k^*(t - t_1) \right) \left(\sum_{l, \omega} e^{-i\omega t/\hbar} S_l(\omega) \otimes \hat{R}_l(t) \right) dt_1 \right] \\ = & -\frac{\alpha^2}{\hbar^2} \text{Tr}_R \left[\int_0^\infty \sum_{k, l, \omega, \omega'} e^{i(\omega' - \omega)t/\hbar} e^{i\omega t_1/\hbar} (S_k^*(\omega') S_l(\omega) \hat{\sigma}(t)) \otimes (\hat{R}_k^*(t) \hat{R}_l(t - t_1) \hat{\rho}(0)) dt_1 \right. \\ & - \int_0^\infty \sum_{k, l, \omega, \omega'} e^{i(\omega' - \omega)t/\hbar} e^{-i\omega' t_1/\hbar} (S_l(\omega) \hat{\sigma}(t) S_k^*(\omega')) \otimes (\hat{R}_l(t) \hat{\rho}(0) \hat{R}_k^*(t - t_1)) dt_1 \\ & - \int_0^\infty \sum_{k, l, \omega, \omega'} e^{i(\omega' - \omega)t/\hbar} e^{i\omega t_1/\hbar} (S_l(\omega) \hat{\sigma}(t) S_k^*(\omega')) \otimes (\hat{R}_l(t - t_1) \hat{\rho}(0) \hat{R}_k^*(t)) dt_1 \\ & \left. + \int_0^\infty \sum_{k, l, \omega, \omega'} e^{i(\omega' - \omega)t/\hbar} e^{-i\omega' t_1/\hbar} (\hat{\sigma}(t) S_k^*(\omega') S_l(\omega)) \otimes (\hat{\rho}(0) \hat{R}_k^*(t - t_1) \hat{R}_l(t)) dt_1 \right] \end{aligned}$$

$$\begin{aligned}
&= \frac{\alpha^2}{\hbar^2} \sum_{k,l,\omega,\omega'} e^{i(\omega'-\omega)t/\hbar} \left[- (S_k^*(\omega') S_l(\omega) \hat{\sigma}(t)) \int_0^\infty e^{i\omega t_1/\hbar} \text{Tr}(\hat{R}_k^*(t) \hat{R}_l(t-t_1) \hat{\rho}(0)) dt_1 \right. \\
&\quad + (S_l(\omega) \hat{\sigma}(t) S_k^*(\omega')) \int_0^\infty e^{-i\omega' t_1/\hbar} \text{Tr}(\hat{R}_k^*(t-t_1) \hat{\rho}(0) \hat{R}_l(t)) dt_1 \\
&\quad + (S_l(\omega) \hat{\sigma}(t) S_k^*(\omega')) \int_0^\infty e^{i\omega t_1/\hbar} \text{Tr}(\hat{R}_l(t-t_1) \hat{\rho}(0) \hat{R}_k^*(t)) dt_1 \\
&\quad \left. - (\hat{\sigma}(t) S_k^*(\omega') S_l(\omega)) \int_0^\infty e^{-i\omega' t_1/\hbar} \text{Tr}(\hat{\rho}(0) \hat{R}_l(t) \hat{R}_k^*(t-t_1)) dt_1 \right]
\end{aligned}$$

Notice that the first and third term combine to be equal to

$$\sum_{k,l,\omega,\omega'} e^{i(\omega'-\omega)t/\hbar} \Gamma_{kl}(\omega) [S_l(\omega) \hat{\sigma}(t), S_k^*(\omega')]. \quad (3.41)$$

Whilst the second and third term combine to be equal to

$$\sum_{k,l,\omega,\omega'} e^{i(\omega'-\omega)t/\hbar} [S_l(\omega), \hat{\sigma}(t) S_k^*(\omega')] \int_0^\infty e^{-i\omega' t_1} \text{Tr}(\hat{R}_k^*(t-t_1) \hat{\rho}(0) \hat{R}_l(t)) dt_1. \quad (3.42)$$

Recall that the reservoir was in a thermal state. Therefore, the Hamiltonian and $\hat{\rho}(0)$ commute. Hence, $\hat{\rho}(0) = \rho(0)$ and we have that

$$\begin{aligned}
\int_0^\infty e^{-i\omega' t_1} \text{Tr}(\hat{R}_k^*(t-t_1) \hat{\rho}(0) \hat{R}_l(t)) dt_1 &= \int_0^\infty e^{-i\omega' t_1} \text{Tr}(e^{iH_R(t-t_1)/\hbar} R_k^* e^{-iH_R(t-t_1)/\hbar} \\
&\quad \rho(0) e^{iH_R t/\hbar} R_l e^{-iH_R t/\hbar}) dt_1 \\
&= \int_0^\infty e^{-i\omega' t_1} \text{Tr}(e^{-iH_R t_1/\hbar} R_k^* e^{iH_R t_1/\hbar} \rho(0) R_l) dt_1 \\
&= \left(\int_0^\infty e^{i\omega' t_1} \text{Tr}(R_l^* e^{iH_R t_1/\hbar} R_k e^{-iH_R t_1/\hbar} \rho(0)) dt_1 \right)^* = \Gamma_{lk}^*(\omega').
\end{aligned}$$

Which completes the proof. ■

3.2.3. THE ROTATING WAVE APPROXIMATION

In this section we derive the Lindblad equation by applying the rotating wave approximation. Which, combined with the propositions and lemmas of the previous section, results in the required Lindblad equation.

One of the approximations that is utilised a lot in physics, for instance in optics, is the rotating wave approximation. It states that any frequency difference that is too great (i.e. $|\omega - \omega'| > \alpha^2$), oscillates too fast to be able to contribute on the timescales that are being considered. Hence, we only want to consider frequencies $\omega' = \omega$. To do this we add a $\delta(\omega - \omega')$ into the expression. This simplification applied to lemma 3.12 yields

$$\frac{d\hat{\sigma}}{dt}(t) = \frac{\alpha^2}{\hbar^2} \sum_{k,l} (\Gamma_{kl}(\omega) [S_l(\omega) \hat{\sigma}(t), S_k^*(\omega)] + \Gamma_{lk}^*(\omega) [S_l(\omega), \hat{\sigma}(t) S_k^*(\omega)]). \quad (3.43)$$

This is the final approximation of this derivation. Hence, we can now state the final lemma.

Lemma 3.13. The evolution of the system from the Redfield equation can be written as

$$\frac{d\sigma}{dt}(t) = -i[H + \frac{\alpha^2}{\hbar^2} H_{LS}, \sigma(t)] + \frac{\alpha^2}{\hbar^2} \sum_{k,l} \gamma_{kl}(\omega) \left(S_l(\omega) \sigma(t) S_k^*(\omega) - \frac{1}{2} \{S_k^* S_l(\omega), \sigma(t)\} \right). \quad (3.44)$$

In this equation the γ_{kl} are all Hermitian and H_{LS} is the Lamb shift Hamiltonian.

Proof. To derive this expression we simply decompose the Γ_{kl} into a Hermitian and non Hermitian part as follows

$$\Gamma_{kl}(\omega) = \frac{1}{2} \gamma_{kl}(\omega) + i\pi_{kl}(\omega), \quad (3.45)$$

$$\pi_{kl} := -\frac{i}{2} (\Gamma_{kl}(\omega) - \Gamma_{kl}^*(\omega)), \quad (3.46)$$

$$\gamma_{kl} := \Gamma_{kl}(\omega) + \Gamma_{kl}^*(\omega). \quad (3.47)$$

This implies that

$$\begin{aligned} \frac{d\hat{\sigma}}{dt}(t) &= \frac{\alpha^2}{\hbar^2} \sum_{k,l} \frac{1}{2} (\gamma_{kl}(\omega) + i\pi_{kl}(\omega)) [S_l(\omega) \hat{\sigma}(t), S_k^*(\omega)] + \frac{1}{2} (\gamma_{kl}(\omega) - i\pi_{kl}(\omega)) [S_l(\omega), \hat{\sigma}(t) S_k^*(\omega)] \\ &= \sum_{k,l} \left[\frac{\alpha^2 i\pi_{kl}}{\hbar^2} ([S_l(\omega) \hat{\sigma}(t), S_k^*(\omega)] - [S_l(\omega), \hat{\sigma}(t) S_k^*(\omega)]) \right] \\ &\quad + \frac{\alpha^2}{\hbar^2} \frac{1}{2} \gamma_{kl}(\omega) ([S_l(\omega) \hat{\sigma}(t), S_k^*(\omega)] + (\omega) [S_l(\omega), \hat{\sigma}(t) S_k^*(\omega)]) \\ &= -i \left[\sum_{k,l} \frac{\alpha^2}{\hbar^2} (\pi_{kl} S_k^* S_l, \hat{\sigma}(t)) \right] + \sum_{k,l} \frac{\alpha^2}{\hbar^2} \gamma_{kl} \left(S_l(\omega) \hat{\sigma}(t) S_k^*(\omega) - \frac{1}{2} \{S_k^*(\omega) S_l(\omega), \hat{\sigma}(t)\} \right) \\ \Rightarrow \frac{d\sigma}{dt}(t) &= -i[H + H_{LS}, \sigma(t)] + \sum_{k,l} \frac{\alpha^2}{\hbar^2} \gamma_{kl} \left(S_l(\omega) \sigma(t) S_k^*(\omega) - \frac{1}{2} \{S_k^*(\omega) S_l(\omega), \sigma(t)\} \right). \end{aligned}$$

Where the last equality follows from transitioning back to the Schrödinger picture and defining the Lamb shift Hamiltonian to be given by $H_{LS} = \sum_{\omega,k,l} \frac{\alpha^2}{\hbar^2} \pi_{kl} S_k^* S_l$. This Hamiltonian is there to renormalize the energy levels after interaction with the environment. ■

This equation already looks like the Lindblad equation, however by employing the fact that that γ_{kl} is Hermitian, we know that we can diagonalize the (γ_{kl}) in some basis, i.e. there exists a unitary operator O such that $O(\gamma_{kl})O^*$ is a diagonal matrix. Therefore, we can write the master equation in a diagonal form yielding

$$\frac{d\sigma}{dt}(t) = -i[H + H_{LS}, \sigma(t)] + \sum_n \frac{\alpha^2}{\hbar^2} \left(L_n(\omega) \sigma(t) L_n^*(\omega) - \frac{1}{2} \{L_n^*(\omega) L_n(\omega), \sigma(t)\} \right). \quad (3.48)$$

Which is exactly the same master equation we derived before using rigorous mathematics. Hence, we see that using several physically motivated approximations, which can be employed in most circumstances, we obtained a similar answer. Thus we can conclude that if our assumptions are valid we have a description that agrees with the mathematics and is therefore at least mathematically valid.

3.3. EXAMPLE: TWO LEVEL SYSTEM

In this short section we will consider an example of the form of the Lindblad equation of a two level system coupled to an energy bath. This energy bath must contain a collection of incoherent oscillators with a continuum of frequencies, which can for instance be phonons close to the qubit.

To start off recall the spin up, spin down basis represented by $e_0 = [0 \ 1]^T$ the ground state and $e_1 = [1 \ 0]^T$ the excited state of a spin 1/2 particle. Furthermore, we have the Pauli matrices given in the following definition.

Definition 3.14. The Pauli matrices are defined as $\sigma_1, \sigma_2, \sigma_3$.

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (3.49)$$

Additionally, the following operators can be defined using the Pauli matrices.

$$\sigma_+ = e_1^* e_0 = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} = \frac{1}{2}(\sigma_1 + i\sigma_2), \quad \sigma_- = e_0^* e_1 = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} = \frac{1}{2}(\sigma_1 - i\sigma_2). \quad (3.50)$$

These operators can be thought of as increasing or decreasing the amount of energy in the system by changing the state of the system. Usually the two level system comes with the Hamiltonian $H = \frac{1}{2}\hbar\omega\sigma_3$, where $\omega > 0$. With this Hamiltonian the interpretation of the σ_+ and σ_- is immediately obvious. Furthermore, the Pauli matrices obey

$$[\sigma_i, \sigma_j] = 2i\varepsilon_{ijk}\sigma_k,$$

where ε_{ijk} is the Levi-Cevita symbol (for further reading see Nielsen and Chuang [21] pages 77-78). Using this framework we can now follow an example as shown in Breuer and Petruccione [5] (pages 146-149).

Proposition 3.15. The Lindblad equation for the two level system is given as

$$\begin{aligned} \frac{d\rho}{dt} = & -\frac{i}{\hbar}[H, \rho(t)] + \gamma_1 \left(\sigma_- \rho(t) \sigma_+ - \frac{1}{2} \sigma_+ \sigma_- \rho(t) - \frac{1}{2} \rho(t) \sigma_+ \sigma_- \right) \\ & + \gamma_2 \left(\sigma_+ \rho(t) \sigma_- - \frac{1}{2} \sigma_- \sigma_+ \rho(t) - \frac{1}{2} \rho(t) \sigma_- \sigma_+ \right). \end{aligned} \quad (3.51)$$

Where the $\gamma_i > 0$.

Proof. Note that the operators σ_- and σ_+ are the eigenfunctions of H . This can be seen by employing the previous commutation relation.

$$[H_S, \sigma_+] = \frac{1}{4}\hbar\omega([\sigma_3, \sigma_1] + i[\sigma_3, \sigma_2]) = \hbar\omega\sigma_+ \quad (3.52)$$

$$[H_S, \sigma_-] = \frac{1}{4}\hbar\omega([\sigma_3, \sigma_1] - i[\sigma_3, \sigma_2]) = -\hbar\omega\sigma_- \quad (3.53)$$

Which yields the Lindblad operators. Hence, setting ρ as the density matrix of the system we have that the Lindblad equation is given as

$$\begin{aligned} \frac{d\rho}{dt} = & -\frac{i}{\hbar} [H, \rho(t)] + \gamma_1 \left(\sigma_- \rho(t) \sigma_+ - \frac{1}{2} \sigma_+ \sigma_- \rho(t) - \frac{1}{2} \rho(t) \sigma_+ \sigma_- \right) \\ & + \gamma_2 \left(\sigma_+ \rho(t) \sigma_- - \frac{1}{2} \sigma_- \sigma_+ \rho(t) - \frac{1}{2} \rho(t) \sigma_- \sigma_+ \right). \end{aligned} \quad (3.54)$$

Here, the γ_i 's represent the coupling to the energy field and also include the spontaneous emission rate and can actually be derived to be given by

$$\begin{aligned} \gamma_1 &= \gamma_0(P(\omega) + 1) \\ \gamma_2 &= \gamma_0 P(\omega). \end{aligned}$$

In these equations $P(\omega)$ is the Planck distribution and γ_0 is the spontaneous emission rate. This can be seen when using the optical version of the Master equation, which we will not look into further (for the interested reader see [5] pages 141-146). ■

Note that we only consider one frequency ω in our Hamiltonian, hence, we set $P = P(\omega)$ for convenience. To see how our system actually behaves we want to solve for the density matrix. To this end consider a convenient way of writing the density matrix, which can easily be seen by writing out the terms.

$$\rho(t) = \frac{1}{2} (I + \langle \vec{n}(t) \rangle \cdot \vec{\sigma}). \quad (3.55)$$

Where, $\vec{n}(t)$ is usually called the Bloch vector. Furthermore, it is easy to prove that $\langle \sigma_i \rangle = \text{Tr}(\sigma_i \rho) = n_i$. This implies that

$$\rho(t) = \frac{1}{2} (I + \langle \vec{\sigma}(t) \rangle \cdot \vec{\sigma}(t)) = \begin{pmatrix} \frac{1}{2}(1 + \langle \sigma_3(t) \rangle) & \langle \sigma_-(t) \rangle \\ \langle \sigma_+(t) \rangle & \frac{1}{2}(1 - \langle \sigma_3(t) \rangle) \end{pmatrix}. \quad (3.56)$$

Using this form of the density matrix we can expand on the example by Breuer and Petrucione [5] (pages to figure out the steady state solution of the system. Given in the following proposition.

Proposition 3.16. The steady state solution for the density matrix of a two level system is given as

$$\frac{1}{2} \begin{pmatrix} 1 - \frac{1}{2^{P+1}} & 0 \\ 0 & 1 + \frac{1}{2^{P+1}} \end{pmatrix}. \quad (3.57)$$

In this equation we neglected the non-dissipative part of the Lindblad equation, because the interesting evolution is contained in the interaction terms.

Proof. For now, only consider the dissipative part of the Lindblad equation. Hence, at the

moment we leave out the non-dissipative part

$$\begin{aligned}
\frac{d\rho}{dt} &= \gamma_0(P+1) \left(\sigma_- \rho(t) \sigma_+ - \frac{1}{2} \sigma_+ \sigma_- \rho(t) - \frac{1}{2} \rho(t) \sigma_+ \sigma_- \right) \\
&\quad + \gamma_0 P \left(\sigma_+ \rho(t) \sigma_- - \frac{1}{2} \sigma_- \sigma_+ \rho(t) - \frac{1}{2} \rho(t) \sigma_- \sigma_+ \right) \\
&= \gamma_0(P+1) \left(\begin{pmatrix} 0 & 0 \\ 0 & \frac{1}{2}(1 + \langle \sigma_3(t) \rangle) \end{pmatrix} - \frac{1}{2} \begin{pmatrix} \frac{1}{2}(1 + \langle \sigma_3(t) \rangle) & 0 \\ \langle \sigma_+(t) \rangle & 0 \end{pmatrix} - \frac{1}{2} \begin{pmatrix} \frac{1}{2}(1 + \langle \sigma_3(t) \rangle) & \langle \sigma_-(t) \rangle \\ 0 & 0 \end{pmatrix} \right) \\
&\quad + \gamma_0 P \left(\begin{pmatrix} \frac{1}{2}(1 - \langle \sigma_3(t) \rangle) & 0 \\ 0 & 0 \end{pmatrix} - \frac{1}{2} \begin{pmatrix} 0 & 0 \\ \langle \sigma_+(t) \rangle & \frac{1}{2}(1 - \langle \sigma_3(t) \rangle) \end{pmatrix} - \frac{1}{2} \begin{pmatrix} 0 & \langle \sigma_-(t) \rangle \\ 0 & \frac{1}{2}(1 - \langle \sigma_3(t) \rangle) \end{pmatrix} \right) \\
&= \begin{pmatrix} -\frac{\gamma_0}{2} - \frac{\gamma_0(2P+1)}{2} \langle \sigma_3(t) \rangle & -\frac{\gamma_0(2P+1)}{2} \langle \sigma_-(t) \rangle \\ -\frac{\gamma_0(2P+1)}{2} \langle \sigma_+(t) \rangle & \frac{\gamma_0}{2} + \frac{\gamma_0(2P+1)}{2} \langle \sigma_3(t) \rangle \end{pmatrix}.
\end{aligned}$$

To properly solve the equation for steady state, we must also consider the non-dissipative part. To this end we calculate the commutator as follows

$$\begin{aligned}
-\frac{i}{\hbar} [H_S, \rho(t)] &= -\frac{i\omega}{2} [\sigma_3, \rho(t)] \\
&= -\frac{i\omega}{2} \left(\begin{pmatrix} \frac{1}{2}(1 + \langle \sigma_3(t) \rangle) & \langle \sigma_-(t) \rangle \\ -\langle \sigma_+(t) \rangle & -\frac{1}{2}(1 - \langle \sigma_3(t) \rangle) \end{pmatrix} - \begin{pmatrix} \frac{1}{2}(1 + \langle \sigma_3(t) \rangle) & -\langle \sigma_- \rangle \\ \langle \sigma_+(t) \rangle & -\frac{1}{2}(1 - \langle \sigma_3(t) \rangle) \end{pmatrix} \right) \\
&= \begin{pmatrix} 0 & i\omega \langle \sigma_-(t) \rangle \\ -i\omega \langle \sigma_+(t) \rangle & 0 \end{pmatrix}
\end{aligned}$$

The combination of the dissipative and non-dissipative part of the Lindblad equation leads to

$$\frac{d\rho}{dt} = \begin{pmatrix} -\frac{\gamma_0}{2} - \frac{\gamma_0(2P+1)}{2} \langle \sigma_3(t) \rangle & \left(i\omega - \frac{\gamma_0(2P+1)}{2} \right) \langle \sigma_-(t) \rangle \\ \left(i\omega - \frac{\gamma_0(2P+1)}{2} \right) \langle \sigma_+(t) \rangle & \frac{\gamma_0}{2} + \frac{\gamma_0(2P+1)}{2} \langle \sigma_3(t) \rangle \end{pmatrix}. \quad (3.58)$$

These matrix equations immediately lead to the following differential equations.

$$\frac{d\langle \sigma_1(t) \rangle}{dt} = \left(i\omega - \frac{\gamma_0(2P+1)}{2} \right) \langle \sigma_1(t) \rangle \quad (3.59)$$

$$\frac{d\langle \sigma_2(t) \rangle}{dt} = \left(i\omega - \frac{\gamma_0(2P+1)}{2} \right) \langle \sigma_2(t) \rangle \quad (3.60)$$

$$\frac{d\langle \sigma_3(t) \rangle}{dt} = -\gamma_0((2P+1) \langle \sigma_3(t) \rangle + 1). \quad (3.61)$$

Which under the steady state assumption yield the solution as proposed above as $\langle \sigma_1(t) \rangle = \langle \sigma_2(t) \rangle = 0$ and $\langle \sigma_3(t) \rangle = -\frac{1}{2P+1}$. Since γ_0, ω and P are all real, we cannot solve $i\omega - \frac{\gamma_0(2P+1)}{2} = 0$, thus we require $\langle \sigma_1(t) \rangle = \langle \sigma_2(t) \rangle = 0$. ■

Finding the steady state solution for the entire equation is the first step in the direction of driven dynamical analysis of a such a system. For times shorter than the time it takes to reach steady state, we still have coherence, which can be seen by solving equations 3.59:3.61 exactly.

This yields the following result

$$\langle \sigma_1(t) \rangle = \exp\left\{\left(i\omega - \frac{\gamma_0(2P+1)}{2}\right)t\right\} \quad (3.62)$$

$$\langle \sigma_2(t) \rangle = \exp\left\{\left(i\omega - \frac{\gamma_0(2P+1)}{2}\right)t\right\} \quad (3.63)$$

$$\langle \sigma_3(t) \rangle = \frac{1}{2P+1} (\exp\{-\gamma_0(2P+1)t\} - 1). \quad (3.64)$$

In these equations we have replaced e^{\cdot} with $\exp\{\cdot\}$ to make the equations more readable. The results in equations 3.62:3.64 in turn give us the density matrix

$$\begin{aligned} \rho &= \begin{pmatrix} \frac{1}{2}(1 + \langle \sigma_3(t) \rangle) & \langle \sigma_-(t) \rangle \\ \langle \sigma_+(t) \rangle & \frac{1}{2}(1 - \langle \sigma_3(t) \rangle) \end{pmatrix} \\ &= \begin{pmatrix} \frac{1}{2}\left(1 + \frac{1}{2P+1}(\exp\{-\gamma_0(2P+1)t\} - 1)\right) & \frac{1}{2} \exp\left\{\left(i\omega - \frac{\gamma_0(2P+1)}{2}\right)t\right\}(1 - i) \\ \frac{1}{2} \exp\left\{\left(i\omega - \frac{\gamma_0(2P+1)}{2}\right)t\right\}(1 + i) & \frac{1}{2}\left(1 - \frac{1}{2P+1}(\exp\{-\gamma_0(2P+1)t\} - 1)\right) \end{pmatrix}. \end{aligned} \quad (3.65)$$

As we can see, for times that are small enough, there is still coherence. That is, the off-diagonal components of the density matrix are still non-zero. However, after sufficient time all coherence of the system dies out in the standard measurement basis, which is expected for systems connected to a heat bath. Coherence "leaks" away to the environment. In this case the combined state of system and environment is still pure, but the system itself has now become a mixed state. Hence, in theory it is possible to reverse the process and obtain the initial state of the system. However, in practice this is impossible due to the size of the environment. This is the reason why the part of the Lindblad equation that does not contain the Hamiltonian is called the dissipative part, i.e. the part of the time evolution that is irreversible.

4

SIMPLIFICATION OF THE LINDBLAD EQUATION

This section covers the derivation of the Lindblad equation in the case of a certain symmetry, namely the commutation of the generator with a member the group of modular automorphisms on $B(\mathcal{H})$. It turns out that in this case the Lindblad equation simplifies a great deal as Carlen and Maas [6] showed in 2017 for finite dimensional matrix algebras. We further investigate whether the same result holds for infinite dimensional Hilbert spaces under the right assumptions. Hence, from this moment on we will not assume that \mathcal{H} is finite anymore. Furthermore, this chapter is cut into four sections. The first section considers the Hilbert-Schmidt operators. These are used to generalise the Lindblad form of Carlen and Maas in section two to an infinite dimensional form by considering the trace class operators with Hilbert-Schmidt norm instead of all bounded operators $B(\mathcal{H})$. In section three we consider the modular automorphisms group, which describes time propagation. Furthermore, we define a new inner product and consider self-adjointness with respect to this inner product. It turns out that in this case the generators defined so far commute with the modular automorphisms. Lastly, in section four we prove our main result: the general form of the Lindblad equation in case this symmetry holds and show that it greatly reduces the complexity of the form.

4.1. HILBERT-SCHMIDT OPERATORS

In this section we define Hilbert-Schmidt operators and prove several key norm inequalities for the trace and Hilbert-Schmidt norm. Additionally, we show a nice correspondence with the trace class operators $\mathcal{L}_1(\mathcal{H})$. Furthermore, we prove the cyclicity of the trace, i.e. $\text{Tr}(UV) = \text{Tr}(VU)$ which holds exactly for these operators. The fact that this does not hold in general is due to the countably infinite dimension of the Hilbert space. This theory is crucial for the next chapter, where we will generalise results pertaining to a nicer form of the Lindblad equation.

4.1.1. DEFINITION AND INEQUALITIES

This part considers the definition of Hilbert-Schmidt operators, whilst also stating and proving multiple inequalities regarding the Hilbert-Schmidt and trace class norms. Additionally, the famous polar decomposition is discussed and proven.

To begin we define the Hilbert-Schmidt norm as in Murphy [19] (pages 59-66) and follow his reasoning to show some elementary statements.

Definition 4.1. Let X be a linear operator on a Hilbert space \mathcal{H} and let E denote the set of orthonormal basis vectors. Then the Hilbert-Schmidt norm is given as

$$\|X\|_2 = \left(\sum_{x \in E} \|Xx\|^2 \right)^{1/2} = \left(\sum_{x \in E} \langle Xx, Xx \rangle \right)^{1/2} = \text{Tr}(X^*X)^{1/2}. \quad (4.1)$$

If an operator X has $\|X\|_2 < \infty$ we call X a Hilbert-Schmidt operator. Furthermore, the space of Hilbert-Schmidt operators is denoted $\mathcal{L}_2(\mathcal{H})$. It turns out this norm is actually independent of the choice of basis.

Proposition 4.2. The Hilbert-Schmidt norm is independent of the choice of basis.

To prove this statement we require the following formalism for working with infinite sums. Let $(x_j)_{j \in J} \subset \mathcal{H}$, then let \mathcal{J} denote the set of all finite subsets of J . We say that $(x_j)_{j \in J}$ is summable if and only if $\sup_{F \in \mathcal{J}} \sum_{j \in F} x_j < \infty$ in this case

$$\sum_{j \in J} x_j = \sup_{F \in \mathcal{J}} \sum_{j \in F} x_j. \quad (4.2)$$

Using this formalism we can prove the proposition.

Proof. Let E and E' both be bases for a Hilbert space \mathcal{H} . Then let $F \subset E$ be a finite. It follows that for a linear Hilbert-Schmidt operator X

$$\begin{aligned} \sum_{y \in F} \|Xy\|^2 &= \sum_{y \in F} \sum_{z \in E'} |\langle Xy, z \rangle|^2 \\ &= \sum_{z \in E'} \sum_{y \in F} |\langle Xy, z \rangle|^2 \\ &\leq \sum_{z \in E'} \|X^*z\|^2. \end{aligned}$$

We thus have obtained $\sum_{y \in E} \|Xy\|^2 \leq \sum_{z \in E'} \|X^*z\|^2$. Employing the fact that $X^{**} = X$ symmetry then implies

$$\sum_{y \in E'} \|Xy\|^2 = \sum_{z \in E} \|Xz\|^2 = \sum_{z \in E} \|X^*z\|^2. \quad (4.3)$$

■

This proposition therefore also implies that $\|X\|_2 = \|X^*\|_2$. One important example of this quadratic trace norm is the following. Suppose we have an orthonormal basis $(e_n)_{n=1}^\infty$ of a Hilbert space \mathcal{H} and let $X \in B(\mathcal{H})$ then we can define $a_{n,m} = \langle Xe_n, e_m \rangle$, which implies that

$$\|X\|_2 = \sqrt{\sum_{m \in \mathbb{N}} \sum_{n \in \mathbb{N}} |a_{n,m}|^2}. \quad (4.4)$$

Which means that any infinite dimensional matrix representation needs to have quadratic absolute summability if the operator is Hilbert-Schmidt. Additionally, we have the following properties of the Hilbert-Schmidt norm.

Proposition 4.3. Let $U, V \in B(\mathcal{H})$ and let $\lambda \in \mathbb{C}$ then

1. $\|U + V\|_2 \leq \|U\|_2 + \|V\|_2$ and $\|\lambda U\|_2 = |\lambda| \|U\|_2$.
2. $\|U\| \leq \|U\|_2$.
3. $\|UV\|_2 \leq \|U\| \|V\|_2$ and $\|UV\|_2 \leq \|U\|_2 \|V\|$.

Proof. The first point is trivial using the triangle inequality and monotonicity of the square root. For the second point it should be noted that this is also rather easy to prove. Let $x \in \mathcal{H}$ be a unit vector, then there is an orthonormal basis E such that $x \in E$. Hence,

$$\|Ux\|^2 \leq \sum_{y \in E} \|Uy\|^2 = \|U\|_2^2. \quad (4.5)$$

The final point can be proven by taking E an orthonormal basis of \mathcal{H} , which then implies that

$$\|UV\|_2^2 = \sum_{y \in E} \|UVy\|^2 \leq \|U\|^2 \sum_{y \in E} \|Vy\|^2 = \|U\|^2 \|V\|_2^2. \quad (4.6)$$

Employing the same reasoning we can obtain the other inequality, which completes the proof. ■

It is interesting to note that the second point implies that if an operator is Hilbert-Schmidt it is automatically part of $B(\mathcal{H})$. However, if an operator is part of $B(\mathcal{H})$ it is not necessarily Hilbert-Schmidt. Aside, from Hilbert-Schmidt operators we can also recall definition 1.21, which stated that an operator was trace class if and only if $\|X\|_1 = \text{Tr}(|X|) < \infty$. Notice that we can write $\text{Tr}(|X|) = \| |X|^{1/2} \|_2^2$. This fact will be used later on, but first note that a similar variant of proposition 4.3 holds for the trace class norm.

Proposition 4.4. Let $U, V \in B(\mathcal{H})$ and let $\lambda \in \mathbb{C}$.

1. $\|U + V\|_1 \leq \|U\|_1 + \|V\|_2$ and $\|\lambda U\|_1 = |\lambda| \|U\|_1$.
2. $\|U\| \leq \|U\|_1 = \|U^*\|_1$.
3. $\|UV\|_1 \leq \|U\|_1 \|V\|$ and $\|UV\|_1 \leq \|U\| \|V\|_1$.

Proof of the inequality. We will prove condition 2 and leave the rest as an exercise for the reader. To this end, we require the result of condition 2 of proposition 4.3, which results in

$$\|U\|_1 = \| |U|^{1/2} \|_2^2 \geq \| |U|^{1/2} \|_2^2 = \| |U| \| = \|U\|. \quad (4.7)$$

To prove the equality we require a bit more theory, which we introduce below. ■

In addition to the theory developed so far, we need the following definition and the lemma of polar decomposition adapted from Van Neerven [26].

Definition 4.5. A partial isometry $V : \mathcal{H} \rightarrow \mathcal{H}$ is a bounded linear operator which is an isometry on the complement of its kernel. Hence, we can decompose the domain of V as $\mathcal{H} = \mathcal{H}_0 \oplus \mathcal{H}_0^\perp$, where V is an isometry on \mathcal{H}_0 and 0 on \mathcal{H}_0^\perp .

To better understand this definition, consider an example.

Example 4.1. Let X be an operator given by

$$X = \sigma_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}. \quad (4.8)$$

Then the initial subspace, i.e. its domain without the kernel is given by $\{0\} \oplus \mathbb{C}$ and its final subspace, i.e. its codomain is given by $\mathbb{C} \oplus \{0\}$.

Lemma 4.6 (Polar decomposition). Consider a bounded linear operator $X \in B(\mathcal{H})$ and set $|X| = (X^*X)^{1/2}$, then X can be written as $X = U|X|$. In this decomposition U is a partial isometry with initial subspace $\overline{\text{range}(|X|)}$ and final subspace $\overline{\text{range}(X)}$.

Proof. We know that for any $x \in \mathcal{H}$ we have

$$\|Xx\|^2 = \langle X^*Xx, x \rangle = \langle |X|x, |X|x \rangle = \||X|x\|. \quad (4.9)$$

This implies that $U : |T| \rightarrow T$ as a linear operator is well-defined and isometric on $\overline{\text{range}(|X|)}$ to $\overline{\text{range}(X)}$, which follows from the continuity of U . Furthermore, we can extend U to be zero everywhere on $\text{range}(|X|)^\perp$, yielding the required result. ■

The polar decomposition is in essence very similar to the way we write complex numbers, since $z \in \mathbb{C}$ can be written as $z = e^{i \arg(z)} |z|$. Lemma 4.6 is very important in the remaining proofs of this section.

Proof of the equality of proposition 4.4. Recall that we are proving $\|U\|_1 = \|U^*\|_1$. To this end, let $U = V|U|$ be the polar decomposition of U . Then,

$$\begin{aligned} |U^*| &= \left(|U^*|^2\right)^{1/2} \\ &= (UU^*)^{1/2} \\ &= (V|U||U|V^*)^{1/2} \\ &= (V|U|V^*V|U|V^*)^{1/2} \\ &= \left((V|U|V^*)^2\right)^{1/2} \\ &= V|U|V^*. \end{aligned}$$

Which implies that

$$\|U^*\|_1 = \text{Tr}(|U^*|) = \text{Tr}(V|U|V^*) = \text{Tr}(V^*U) = \text{Tr}(|U|) = \|U\|_1. \quad (4.10)$$

This completes the proof. ■

In this proof we used the cyclicity of the trace. However, this does not hold for all operators anymore, since we are working with infinite dimensional Hilbert spaces. Due to the fact that the Hilbert space is countably infinite dimensional, the trace of an operator is not properly defined for most operators. Hence, cyclicity need not hold, since this can yield a divergent trace. Luckily, it does still work for Hilbert-Schmidt operators and trace class operators, which we will prove later in this section. Furthermore, combining two Hilbert-Schmidt operators U_1, U_2 into an operator $V = U_1^* U_2$ does not necessarily yield a Hilbert-Schmidt operator, but this operator has the following nice property.

Lemma 4.7. Let $U_1, U_2 \in \mathcal{L}_2(\mathcal{H})$ and let E be an orthonormal basis of \mathcal{H} . Set $V = U_1^* U_2$. Then $\sum_{x \in E} |\langle V(x), x \rangle| < \infty$ and

$$\sum_{y \in E} \langle Vy, y \rangle = \frac{1}{4} \sum_{k=1}^3 i^k \left\| U_2 + i^k U_1 \right\|_2^2. \quad (4.11)$$

Proof. The first part of the proof can be proven by employing the fact that both U_1 and U_2 are Hilbert-Schmidt operators. Letting $F \subset E$ be non-empty yields

$$\begin{aligned} \sum_{y \in F} |\langle Vy, y \rangle| &= \sum_{y \in F} |\langle U_2 y, U_1 y \rangle| \\ &\leq \sum_{y \in F} \|U_2 y\| \|U_1 y\| \\ &\leq \sqrt{\sum_{y \in F} \|U_2 y\|^2} \sqrt{\sum_{y \in F} \|U_1 y\|^2} < \infty. \end{aligned}$$

Where we used the Cauchy-Schwarz inequality for the last step and recognise that the last terms are exactly the Hilbert-Schmidt norms of U_1 and U_2 . We continue on with the second part for which we require the polarisation identity, given as

$$\langle x, y \rangle = \frac{1}{4} \left(\|x + y\|^2 - \|x - y\|^2 + i(\|x + iy\|^2 - \|x - iy\|^2) \right) = \frac{1}{4} \sum_{k=0}^3 i^k \|x + i^k y\|^2. \quad (4.12)$$

This equation can be obtained by simply writing out each of the norms in terms of inner products and cancelling out multiple terms. Furthermore, employing this identity

$$\begin{aligned} \sum_{y \in E} \langle Vy, y \rangle &= \sum_{y \in E} \langle U_2 y, U_1 y \rangle \\ &= \sum_{y \in E} \frac{1}{4} \sum_{k=0}^3 i^k \left\| U_2 y + i^k U_1 y \right\|^2 \\ &= \frac{1}{4} \sum_{k=0}^3 i^k \sum_{y \in E} \left\| (U_2 + i^k U_1) y \right\|^2 \\ &= \frac{1}{4} \sum_{k=0}^3 i^k \left\| U_2 + i^k U_1 \right\|_2^2, \end{aligned}$$

as required. ■

4.1.2. CORRESPONDENCE BETWEEN TRACE CLASS AND HILBERT-SCHMIDT OPERATORS

This subsection concerns the nice correspondence between the trace class operators and Hilbert-Schmidt operators. Furthermore, the cyclicity of the trace is proven for these two classes of operators. Lastly, an example showcasing the fact that being trace class is a stricter requirement is shown and explained.

We begin with the correspondence, which is captured in the following theorem.

Theorem 4.8. Let X be a linear operator on a Hilbert space \mathcal{H} , then the following are equivalent

1. X is trace class.
2. $|X|$ is trace class.
3. $|X|^{1/2}$ is Hilbert-Schmidt.
4. There exist Hilbert-Schmidt operators U_1 and U_2 on \mathcal{H} such that $X = U_1^* U_2$.

Proof. As can be seen in the discussion above $1 \implies 2$ and $2 \implies 3$ are trivial by looking at the definition of the trace norm. Furthermore, we can prove $3 \implies 4$ by noting that taking $U_1 = U|X|^{1/2}$ and $U_2 = |X|^{1/2}$ with U a partial isometry as defined in lemma 4.6. Then $\|U_1\|_2^2 = \text{Tr}((U|X|^{1/2})^* U|X|^{1/2}) = \text{Tr}((|X|^{1/2})^* |X|^{1/2}) = \| |X|^{1/2} \|_2^2$. Therefore, by the assumption it follows that U_1 and U_2 are Hilbert-Schmidt. Lastly, we have to prove $4 \implies 1$.

To this end, assume $X = U_1 U_2$ with $U_1, U_2 \in \mathcal{L}_2(\mathcal{H})$. If we apply the polar decomposition we obtain $|X| = V^* X = V^* U_1 U_2$. Notice that

$$\|V^* U_1\|_2^2 = \text{Tr}((V^* U_1)^* V^* U_1) = \text{Tr}(U_1^* U_1) = \|U_1\|_2^2. \quad (4.13)$$

Thus by lemma 4.7 we have that

$$\sum_{y \in E} |\langle |X|y, y \rangle| < \infty. \quad (4.14)$$

Therefore, we also have regular convergence and we have that $\| |X| \|_1 < \infty$, thus X is trace class. ■

The polarisation identity and previous theorem can be used to prove the cyclicity of the trace as follows.

Proposition 4.9. Let U and V in $B(\mathcal{H})$. Then $\text{Tr}(UV) = \text{Tr}(VU)$ if either

1. U and V are both Hilbert-Schmidt operators,
2. or V is trace class.

Proof. We split the cases into two parts. For case 1 we can apply the polarisation identity (lemma 4.7) to obtain

$$\text{Tr}(UV) = \frac{1}{4} \sum_{k=1}^3 i^k \|V + i^k U^*\|_2^2$$

$$\begin{aligned}
&= \frac{1}{4} \sum_{k=0}^3 i^k \left\| (V + i^k U^*)^* \right\|_2^2 \\
&= \frac{1}{4} \sum_{k=0}^3 i^k \left\| U + i^k V^* \right\|_2^2 \\
&= \frac{1}{4} \sum_{k=0}^3 i^k \left\| U + i^k V^* \right\|_2^2 \\
&= \text{Tr}(VU).
\end{aligned}$$

In the second equality we applied the fact that $\|U\|_2 = \|U^*\|_2$ from proposition 4.2. If we now consider case 2, we can apply the previous theorem, which implies that there exist operators $U_1, U_2 \in \mathcal{L}_2(\mathcal{H})$ such that $V = U_1 U_2$. This fact can then be used as follows

$$\text{Tr}(UV) = \text{Tr}((U U_1) U_2) = \text{Tr}((U_2 U) U_1) = \text{Tr}(U_1 U_2 U) = \text{Tr}(VU).$$

In this equation we applied the fact that a Hilbert-Schmidt operator multiplied with a bounded operator is again Hilbert-Schmidt. This can be seen as follows by applying theorem 4.3,

$$\|UV\| \leq \|U\|_2 \|V\| < \infty. \quad (4.15)$$

■

Lastly, it should be noted that being trace class is a much stronger assumption than being Hilbert-Schmidt. This can be seen in the following example.

Example 4.2. Let X be the operator defined as

$$X = \begin{pmatrix} 1 & & & & \\ & \frac{1}{2} & & & \\ & & \ddots & & \\ & & & \frac{1}{n} & \\ & & & & \ddots \end{pmatrix}, \quad X^* X = X^2 = \begin{pmatrix} 1 & & & & \\ & \frac{1}{4} & & & \\ & & \ddots & & \\ & & & \frac{1}{n^2} & \\ & & & & \ddots \end{pmatrix}. \quad (4.16)$$

Notice that $\text{Tr}(|X|) = \sum_{n=1}^{\infty} \frac{1}{n}$, which diverges. While $\text{Tr}(X^* X) = \sum_{n=1}^{\infty} \frac{1}{n^2} < \infty$. Hence, being Hilbert-Schmidt does not ensure being trace class. Thus being trace class is a stronger assumption than being Hilbert-Schmidt.

This can also be seen by the fact that theorem 4.8 implies that for every trace class operator X there exist U_1, U_2 both Hilbert-Schmidt such that $X = U_1^* U_2$. Then, the product of Hilbert-Schmidt operators is again Hilbert-Schmidt, which can be seen by applying proposition 4.3 as follows

$$\|X\|_2 = \|U_1^* U_2\|_2 \leq \|U_1^*\|_2 \|U_2\| \leq \|U_1\|_2 \|U_2\|_2 < \infty. \quad (4.17)$$

4.2. GENERALISATIONS TO INFINITE DIMENSIONAL HILBERT SPACES

This section covers the derivation of the Lindblad equation in terms of the GKS matrix, for an infinite dimensional Hilbert space. To generalise the Lindblad equation we will use a special

case of the Hilbert-Schmidt operators, namely the trace class operators with Hilbert-Schmidt norm, instead of the bounded operators, for which the Lindblad form is described in Chapter 3. The first part of this section considers the decomposition of an operator on these operators in terms of the GKS matrix and a generalisation of Choi's theorem regarding the Choi matrix, whilst the second part considers the derivation of the Lindblad equation for generators defined on this special case.

4.2.1. GKS DECOMPOSITION AND GENERALISATION OF THE CHOI-MATRIX THEOREM

This section covers the generalisation of the GKS decomposition for operators on a special case of the trace class operators. Additionally, it covers the generalisation of the theorem of Choi stating that the Choi matrix is positive if and only if the corresponding operator is CP.

To start let $(e_i)_{i \in J} \subset \mathcal{H}$ be an orthonormal basis of \mathcal{H} , where J is a, possibly countable infinite, index set. Furthermore, to define a generator as we did before, where we required $LI = 0$ and $LX^* = (LX)^*$, we need to add the identity operator artificially to the operators of interest. The operators of interest in this case are the trace class operators with a Hilbert-Schmidt norm, denoted $\mathcal{L}_2(\mathcal{H})'$. We take the trace class operators to prevent issues with the convergence of the trace. This latter fact follows from example 4.2, where we saw that not every Hilbert-Schmidt operator is trace class. Hence, adding in the identity operator would lead to infinite traces after taking the inner product. Thus we define the new space as follows.

Definition 4.10. Let $\mathcal{L}_3(\mathcal{H})$ be the space defined by

$$\mathcal{L}_3(\mathcal{H}) = \mathcal{L}_2(\mathcal{H})' \oplus \{\lambda I : \lambda \in \mathbb{C}\}, \quad (4.18)$$

where $\mathcal{L}_2(\mathcal{H})'$ is defined by taking $\mathcal{L}_1(\mathcal{H})$ and taking the closure with respect to the $\|\cdot\|_2$ norm. However, we will normally work with the dense subset $\mathcal{L}_1(\mathcal{H}) \oplus \{\lambda I : \lambda \in \mathbb{C}\}$, such that the trace is defined. Therefore, if we write $\mathcal{L}_3(\mathcal{H})$ we usually mean the dense subset, the same holds for $\mathcal{L}_2(\mathcal{H})'$, normally we will work with $\mathcal{L}_1(\mathcal{H})$ with an inner product structure to make sure the traces of operators are defined. Hence, we also endow $\mathcal{L}_3(\mathcal{H})$ with an inner product defined as follows

$$\langle X, Y \rangle = \begin{cases} \text{Tr}(X^* Y) & X, Y \in \mathcal{L}_2(\mathcal{H})', \\ 0 & X = \lambda I \text{ and } Y \in \mathcal{L}_2(\mathcal{H})' \text{ or } X \in \mathcal{L}_2(\mathcal{H})' \text{ and } Y = \lambda I \text{ for } \lambda \in \mathbb{C}, \\ \bar{\lambda} \mu & X = \lambda I \text{ and } Y = \mu I \text{ for } \lambda, \mu \in \mathbb{C}. \end{cases} \quad (4.19)$$

Notice that this inner product allows us to state that I is orthogonal with respect to $\mathcal{L}_2(\mathcal{H})'$. This is because of the fact that we need to be able to pick an orthonormal basis for $\mathcal{L}_2(\mathcal{H})'$, but this is not possible if the identity is part of the space. Since in this case any operator with non-zero trace would not have a proper decomposition into orthonormal basisvectors of $\mathcal{L}_3(\mathcal{H})$ as soon as we set the first basisvector to be equal to I , which is required for the derivation. Hence, this construction looks a little strange. As mentioned in the discussion of this thesis, it must be looked at whether we can lift these restrictions on the inner product to obtain a more "natural" inner product. Furthermore, we "normalised" the inner product for the case that both X and Y are the identity. The reason we are defining the space in this way results

from the fact that for the generator of a QMS we require $LI = 0$. However, the operators of interest are not equal to the identity. Hence, to keep the two spaces separate and do a proper derivation it is important to prevent operators moving from the regular inner product to the identity, i.e. $LX \neq I$ for all $X \in \mathcal{L}_2(\mathcal{H})'$. Thus, we need to check whether L preserves $\mathcal{L}_2(\mathcal{H})'$. However, before we can do this, we need to redefine the space of operators in a similar way as we defined $\mathcal{L}_3(\mathcal{H})$. This follows from the fact that the space $\mathcal{L}_2(\mathcal{L}_3(\mathcal{H}))$ also needs an identity to prove the supporting results of this thesis. To this end consider the following definition.

Definition 4.11. Let $\mathcal{L}_4(\mathcal{L}_3(\mathcal{H}))$ be defined by

$$\mathcal{L}_4(\mathcal{L}_3(\mathcal{H})) = \mathcal{L}_2(\mathcal{L}_3(\mathcal{H})) \oplus \{\lambda I : \lambda \in \mathbb{C}\}. \quad (4.20)$$

We additionally define the following inner product analogously to the case $\mathcal{L}_3(\mathcal{H})$ as follows

$$\langle X, Y \rangle = \begin{cases} \text{Tr}(X^* Y) & X, Y \in \mathcal{L}_2(\mathcal{L}_3(\mathcal{H})), \\ 0 & X = \lambda I \text{ and } Y \in \mathcal{L}_2(\mathcal{L}_3(\mathcal{H})) \text{ or } X \in \mathcal{L}_2(\mathcal{L}_3(\mathcal{H})) \text{ and } Y = \lambda I \text{ for } \lambda \in \mathbb{C}, \\ \bar{\lambda} \mu & X = \lambda I \text{ and } Y = \mu I \text{ for } \lambda, \mu \in \mathbb{C}. \end{cases} \quad (4.21)$$

Hence, we again defined I to be orthogonal to the other operators in $\mathcal{L}_4(\mathcal{L}_3(\mathcal{H}))$. It should be noted that we only add the identity to prove an important claim later on, for which we need to have defined the inner product properly. However, the final form of the Lindblad equation for generators of QMS is of course never defined for $L = I$, since this case does not satisfy one of the generator requirements ($LI = 0$). Hence, for most purposes the reader can think of $\mathcal{L}_4(\mathcal{L}_3(\mathcal{H}))$ as $\mathcal{L}_2(\mathcal{L}_3(\mathcal{H}))$.

Now that we have the setting of the spaces in which we will be working, we check whether $L \in \mathcal{L}_4(\mathcal{L}_3(\mathcal{H}))$ preserves $\mathcal{L}_3(\mathcal{H})$ under the right assumptions. To this end, consider the following proposition.

Proposition 4.12. Let $L \in \mathcal{L}_4(\mathcal{L}_3(\mathcal{H}))$ be an operator with $LI = 0$. Furthermore, assume that L is self-adjoint. Then L preserves $\mathcal{L}_2(\mathcal{H})'$.

Proof. Let $X \in \mathcal{L}_2(\mathcal{H})'$. Then we know that $\text{Tr}(X) < \infty$. Furthermore, we can write

$$\text{Tr}(LX) = \text{Tr}(I^* LX) = \text{Tr}(L^*(I^*)X) = \text{Tr}(L(I)X) = \text{Tr}(0X) = 0 < \infty. \quad (4.22)$$

Hence, every operator that was in $\mathcal{L}_2(\mathcal{H})'$ remains in $\mathcal{L}_2(\mathcal{H})'$ and the identity gets mapped to the zero operator. \blacksquare

Thus if the generator of a QMS is self-adjoint, then it also preserves the space $\mathcal{L}_2(\mathcal{H})'$. It should be noted that self-adjointness might not seem well-defined due to the redefinition of the inner product. However, for both $X, Y \in \mathcal{L}_2(\mathcal{H})'$ $\langle X, Y \rangle$ is well-defined. Furthermore, suppose $X = I$. Then $\langle X, LY \rangle = \langle I, LY \rangle = 0$, which should be the same as $\langle LX, Y \rangle = \langle LI, Y \rangle = \langle 0, Y \rangle = \text{Tr}(0Y) = 0$. Hence, this does not lead to any issues. With similar reasoning it can be shown that this is also the case for $Y = I$. Additionally, suppose both $X = I$ and $Y = I$, then $\langle LX, Y \rangle = \langle LI, I \rangle = 0 = \langle I, LI \rangle$. Therefore, in all cases the self-adjointness works properly.

We have proven that $L \in \mathcal{L}_4(\mathcal{L}_3(\mathcal{H}))$ with L self-adjoint and satisfying the requirements of a QMS generator preserves $\mathcal{L}_2(\mathcal{H})'$. Besides this fact it is interesting to further investigate

$\mathcal{L}_4(\mathcal{L}_3(\mathcal{H}))$. It turns out that there is a nice identification between $\mathcal{L}_4(\mathcal{L}_3(\mathcal{H}))$ and $\mathcal{L}_3(\mathcal{H}) \otimes \mathcal{L}_3(\mathcal{H})$. To prove this fact we make use of the basis for $\mathcal{L}_3(\mathcal{H})$ as follows, we define $E_{i,j} = e_i e_j^*$ for any combination of $i, j \in J$, which is an orthonormal basis of $\mathcal{L}_2(\mathcal{H})'$, since it is a rank one projection. To properly have a basis for the entire space $\mathcal{L}_3(\mathcal{H})$ we add in the identity, which yields an orthonormal basis of $\mathcal{L}_3(\mathcal{H})$.

Definition 4.13. The operator $\#(A \otimes B) : \mathcal{L}_3(\mathcal{H}) \rightarrow \mathcal{L}_3(\mathcal{H})$ for operators $A, B \in \mathcal{L}_3(\mathcal{H})$ is defined as

$$\#(A \otimes B)(X) = AXB, \quad \text{for all } X \in \mathcal{L}_3(\mathcal{H}). \quad (4.23)$$

Furthermore, notice that the trace is given as $\text{Tr}(\#(A \otimes B)) = \text{Tr}(A)\text{Tr}(B)$ except for $A = I$ or $B = I$, since in this case the trace is divergent. To see this, consider the following: let $A, B \in \mathcal{L}_2(\mathcal{H})'$ then there are two ways to compute AXB for some $X \in \mathcal{L}_2(\mathcal{H})'$. We can either do the computation directly or we can unravel X into a column vector \hat{X} . In the latter case we consider $(A \otimes B^T)\hat{X}$ instead of AXB . After the operator $(A \otimes B^T)$ has acted on \hat{X} , we can transform the result from a column vector back to a matrix. The result of both these operations is the same. However, the trace of $A \otimes B^T$ is easily computed as

$$\text{Tr}(A \otimes B^T) = \text{Tr}(A) \text{Tr}(B^T) = \text{Tr}(A) \text{Tr}(B). \quad (4.24)$$

In the first equation we used the fact that the trace of the tensor product is given by the two separate traces. Hence, this is a nice identification to get our required result. To see that this other way of looking at the product AXB actually works we have written out the argument for 2×2 matrices in Appendix B. With this knowledge we can now state the first lemma.

Lemma 4.14. Let F_α and G_β be two orthonormal bases for $\mathcal{L}_3(\mathcal{H})$ such that $F_1 = G_1 = I$. Additionally, $\{F_\alpha \otimes G_\beta\}_{\alpha, \beta \neq 1} \cup \{F_1 \otimes G_1\}$ is an orthonormal set in $\mathcal{L}_3(\mathcal{H}) \otimes \mathcal{L}_3(\mathcal{H})$. Then $\{\#(F_\alpha \otimes G_\beta)\}_{\alpha, \beta \neq 1} \cup \{\#(F_1 \otimes G_1)\}$ is an orthonormal set in $\mathcal{L}_4(\mathcal{L}_3(\mathcal{H}))$.

Proof. We will first focus on the part of the basis of $\mathcal{L}_2(\mathcal{H})'$. Hence, we currently leave out the identity or F_1 and G_1 . This yields

$$\begin{aligned} \langle \#(F_\alpha \otimes G_\beta), \#(F_\mu \otimes G_\nu) \rangle_{\mathcal{L}_4(\mathcal{L}_3(\mathcal{H}))} &= \text{Tr}(\#(F_\alpha \otimes G_\beta)^* \#(F_\mu \otimes G_\nu)) \\ &= \text{Tr} \left(\sum_{i,j \in J} (F_\alpha E_{i,j} G_\beta)^* (F_\mu E_{i,j} G_\nu) \right) \\ &= \sum_{i,j \in J} \text{Tr}((F_\alpha E_{i,j} G_\beta)^* (F_\mu E_{i,j} G_\nu)). \end{aligned}$$

We can pull out the summation, because the product of two Hilbert-Schmidt operators is again Hilbert-Schmidt and all trace class operators are Hilbert-Schmidt:

$$\|UV\|_2 \leq \|U\| \|V\|_2 \leq \|U\|_2 \|V\|_2, \quad (4.25)$$

by the norm inequality $\|U\| \leq \|U\|_2$ and the identity $\|UV\|_2 \leq \|U\| \|V\|_2$. Furthermore, we know that the trace of trace class operators converges absolutely and the product of trace

class operators is again trace class by proposition 4.4. Hence, interchanging order of summation is allowed. We continue on as follows by working out the adjoint and applying the cyclic property of the trace for trace class operators

$$\begin{aligned} \sum_{i,j \in J} \text{Tr}((F_\alpha E_{i,j} G_\beta)^* (F_\mu E_{i,j} G_\nu)) &= \sum_{i,j \in J} \text{Tr}(G_\beta^* E_{j,i} F_\alpha^* (F_\mu E_{i,j} G_\nu)) \\ &= \sum_{i,j \in J} \langle G_\nu G_\beta^* e_j, e_j \rangle \langle F_\alpha^* F_\mu e_i, e_i \rangle \\ &= \text{Tr}(G_\nu G_\beta^*) \text{Tr}(F_\mu F_\alpha^*) = \delta_{\nu,\beta} \delta_{\mu,\alpha}. \end{aligned}$$

Hence, the elements are orthonormal. However, we have not included the identity yet. Notice that $\#(I \otimes I) = I_{\mathcal{L}_4(\mathcal{L}_3(\mathcal{H}))}$. Hence, $\langle \#(I \otimes I), X \rangle \neq 0$ if and only if $X = I$ by definition. Thus we have added an extra element to the orthonormal set, which precisely covers $I \in \mathcal{L}_4(\mathcal{L}_3(\mathcal{H}))$. Therefore, the union of this element with $\#(F_\alpha \otimes G_\beta)|_{\alpha,\beta \neq (1,1)}$ yields an orthonormal set of $\mathcal{L}_4(\mathcal{L}_3(\mathcal{H}))$. \blacksquare

Notice that the previous lemma nearly constructs an equivalence between orthonormal bases. We have $\mathcal{L}_2(\mathcal{L}_2(\mathcal{H})') \simeq \mathcal{L}_2(\mathcal{H})' \otimes \mathcal{L}_2(\mathcal{H})'$ and $I_{\mathcal{L}_4(\mathcal{L}_3(\mathcal{H}))} \simeq I_{\mathcal{L}_3(\mathcal{H})} \otimes I_{\mathcal{L}_3(\mathcal{H})}$. However, the parts of the space defined by $I \otimes \mathcal{L}_2(\mathcal{H})'$ and $\mathcal{L}_2(\mathcal{H})' \otimes I$ do not get identified with an element $\#(I \otimes X)$ or $\#(X \otimes I)$ for $X \in \mathcal{L}_2(\mathcal{H})'$. This has to do with the fact that these vectors are not orthonormal, to the vectors stated in the lemma. This can be seen by considering the same derivation as in the lemma. Recall the following identity

$$\langle \#(F_\alpha \otimes G_\beta), \#(F_\mu \otimes G_\nu) \rangle_{\mathcal{L}_2(\mathcal{L}_3(\mathcal{H}))} = \text{Tr}(G_\nu G_\beta^*) \text{Tr}(F_\mu F_\alpha^*). \quad (4.26)$$

Using this identity we can consider the case $\#(F_1 \otimes G_\beta) = \#(I \otimes G_\beta)$, where $G_\beta \neq I$, then

$$\langle \#(I \otimes G_\beta), \#(F_\mu \otimes G_\nu) \rangle_{\mathcal{L}_2(\mathcal{L}_3(\mathcal{H}))} = \text{Tr}(G_\nu G_\beta^*) \text{Tr}(F_\mu) \neq \delta_{\nu,\beta} \delta_{\mu,\alpha} \quad \text{if } F_\mu \text{ is not traceless.} \quad (4.27)$$

We see that if F_μ is not traceless we do not have the same nice identification. Furthermore, since we have defined I orthogonal to all elements in $\mathcal{L}_2(\mathcal{H})'$ we cannot choose a basis that has F_μ traceless for all $\mu \neq 1$. Thus, we cannot use the identification of $\mathcal{L}_2(\mathcal{L}_3(\mathcal{H}))$ and $\mathcal{L}_3(\mathcal{H}) \otimes \mathcal{L}_3(\mathcal{H})$ in this case. However, we would like to decompose operators into a sum of orthonormal projections. To this end, suppose we have an arbitrary operator $L \in \mathcal{L}_4(\mathcal{L}_3(\mathcal{H}))$, then let $\{F_\mu\}$ be an orthonormal basis of $\mathcal{L}_3(\mathcal{H})$. It is then easy to see that $\{F_\mu^*\}$ is also an orthonormal basis of $\mathcal{L}_3(\mathcal{H})$. Now if lemma 4.14 constructed an orthonormal basis instead of just an orthonormal set, we could write an orthonormal decomposition as

$$L = \sum_{\alpha,\beta} c_{\alpha,\beta} \#(F_\alpha^* \otimes F_\beta). \quad (4.28)$$

In this equation the $c_{\alpha,\beta} = \langle \#(F_\alpha^* \otimes F_\beta), L \rangle_{\mathcal{L}_4(\mathcal{L}_3(\mathcal{H}))}$ i.e. the projection of L onto the basis vector $\#(F_\alpha^* \otimes F_\beta)$. This is very similar to decomposing a matrix as A as $A = \sum_{i,j} A_{i,j} E_{i,j}$. However, notice that we have also included terms with $\#(I \otimes F_\beta)$, which are not orthonormal vectors. Thus, the decomposition would not be a proper orthogonal decomposition. Hence, we

set the elements $c_{(1,1),\beta} = c_{\beta,(1,1)} = 0$ for all β , which allows us to just consider the orthonormal set. It is not immediately obvious why we are allowed to do this, but it is convenient. Furthermore, it turns out that for the operators of interest this assumption is actually true. This will be shown later on.

Definition 4.15. The operator $c_{\alpha,\beta}$ with $\alpha, \beta \in J$ with $c_{\alpha,\beta} = \langle \#(F_\alpha^* \otimes F_\beta), L \rangle_{\mathcal{L}_4(\mathcal{L}_3(\mathcal{H}))}$ is called the GKS-matrix.

An important property of the GKS-matrix is that the expansion of L is unique, because it is made up out of the projection of orthonormal vectors for the non-zero components. We can now continue with the following lemma, which should immediately be recognised as a symmetry obtained from the fact that our generator is a $*$ -map.

Lemma 4.16. Let $L \in \mathcal{L}_4(\mathcal{L}_3(\mathcal{H}))$ and let $\{F_\alpha\}$ be an orthonormal basis of $\mathcal{L}_3(\mathcal{H})$. Then the GKS-matrix of L with respect to the basis is self-adjoint if and only if L is a $*$ -map, i.e. $L(X)^* = L(X^*)$ for all $X \in \mathcal{L}_2(\mathcal{H})$.

Proof. Let $L = \sum_{\alpha,\beta} c_{\alpha,\beta} \#(F_\alpha^* \otimes F_\beta)$ defining $\tilde{L}(X) = (L(X^*))^*$ then yields

$$\tilde{L}(X) = \left(\sum_{\alpha,\beta} c_{\alpha,\beta} F_\alpha^* X^* F_\beta \right)^* = \sum_{\alpha,\beta} \overline{c_{\alpha,\beta}} F_\beta^* X F_\alpha = \sum_{\alpha,\beta} \overline{c_{\beta,\alpha}} F_\alpha^* X F_\beta. \quad (4.29)$$

Because the expansion is unique, we have that $\tilde{L} = L$ if and only if $c_{\alpha,\beta} = \overline{c_{\beta,\alpha}}$, which completes the proof. \blacksquare

To make further use of our GKS-matrix we would ideally like to define another operator, which acts on $\mathcal{L}_3(\mathcal{H})$ such that we can use that space, instead of our more complicated $\mathcal{L}_4(\mathcal{L}_3(\mathcal{H}))$. The following definition in combination with the next lemma is such a result.

Definition 4.17. The Choi matrix of a linear operator $L \in \mathcal{L}_2(\mathcal{L}_2(\mathcal{H})')$ is given by

$$\mathcal{C}(L) = \sum_{i,j \in J} L(E_{i,j}) \otimes E_{i,j}. \quad (4.30)$$

Notice that in this definition leaves out the identity out of both $\mathcal{L}_4(\mathcal{L}_3(\mathcal{H}))$ and $\mathcal{L}_3(\mathcal{H})$. This reduces both spaces back to proper Hilbert spaces. Hence, we can state the following lemma.

Lemma 4.18. Let $L \in \mathcal{L}_2(\mathcal{L}_2(\mathcal{H})')$, and let $\mathcal{C}(L)$ be the Choi matrix. If we now identify $\mathcal{H} \otimes \mathcal{H}$ with $\mathcal{L}_2(\mathcal{H})'$, i.e. we leave out the identity, by using $v \otimes w \mapsto \sum_{i,j \in J} v_i w_j E_{i,j}$. Then, we have that $\mathcal{C}(L)$ is an operator on $\mathcal{L}_2(\mathcal{H})'$, for all $F, G \in \mathcal{L}_2(\mathcal{H})'$. Using this identification we can then show

$$\langle G, \mathcal{C}(L)F \rangle_{\mathcal{L}_2(\mathcal{H})'} = \langle \#(G \otimes F^*), L \rangle_{\mathcal{L}_2(\mathcal{L}_2(\mathcal{H})')}. \quad (4.31)$$

Proof. Note that

$$\langle G, \mathcal{C}(L)F \rangle_{\mathcal{L}_2(\mathcal{H})} = \text{Tr}(G^* \mathcal{C}(L)F)$$

$$\begin{aligned}
&= \text{Tr} \left(G^* \left(\sum_{i,j \in J} L(E_{i,j}) \otimes E_{i,j} \right) F \right) \\
&= \text{Tr} \left(G^* \left(\sum_{i,j \in J} L(E_{i,j}) \otimes E_{i,j} \right) \left(\sum_{l,p \in J} F_{l,p} e_l \otimes e_p \right) \right) \\
&= \text{Tr} \left(G^* \left(\sum_{i,j \in J} \sum_{l,p \in J} F_{l,p} L(E_{i,j}) e_l \otimes E_{i,j} e_p \right) \right) \\
&= \left\langle \sum_{k,m \in J} G_{k,m} e_k \otimes e_m, \sum_{i,j \in J} \sum_{l,p \in J} F_{l,p} L(E_{i,j}) e_l \otimes E_{i,j} e_p \right\rangle.
\end{aligned}$$

Where we defined $X_{i,j} = \langle e_i, X e_j \rangle$ for both F and G . Additionally, in the last equality we used the fact that $\text{Tr}(G^* F) = \langle G, F \rangle$. Furthermore, to pull out the infinite summations note that the inner product is a continuous function with respect to the norm topology, since it is bounded. This can be seen as follows, both G and F are Hilbert-Schmidt operators. Additionally, L is also Hilbert-Schmidt, which implies that all products are also Hilbert-Schmidt by equation 4.25. Hence, letting $y, (x_n)_{n \in \mathbb{N}} \in \mathcal{H}$ we can use the following equality

$$\left\langle y, \sum_{n \in \mathbb{N}} x_n \right\rangle = \left\langle y, \lim_{N \rightarrow \infty} \sum_{n=1}^N x_n \right\rangle = \lim_{N \rightarrow \infty} \sum_{n=1}^N \langle y, x_n \rangle = \sum_{n \in \mathbb{N}} \langle y, x_n \rangle. \quad (4.32)$$

The same reasoning also works for the first argument. This equation leads us to

$$\begin{aligned}
\sum_{k,m \in J} \sum_{i,j \in J} \sum_{l,p \in J} \langle G_{k,m} e_k \otimes e_m, F_{l,p} L(E_{i,j}) e_l \otimes E_{i,j} e_p \rangle &= \sum_{k,m,i,j,l,p \in J} \overline{G_{k,m}} F_{l,p} \langle e_k \otimes e_m, L(E_{i,j}) e_l \otimes E_{i,j} e_p \rangle \\
&= \sum_{k,m,i,j,l,p \in J} \overline{G_{k,m}} F_{l,p} \langle e_k, L(E_{i,p}) e_l \rangle \langle e_m, E_{i,j} e_p \rangle \\
&= \sum_{k,m,i,j,l,p \in J} \overline{G_{k,m}} F_{l,p} L(E_{i,j})_{k,l} (E_{i,j})_{m,p} \\
&= \sum_{k,m,i,j,l,p \in J} F_{l,p} (E_{j,i})_{m,p} \overline{G_{k,m}} L(E_{i,j})_{k,l} \\
&= \sum_{k,i,j,l \in J} (F E_{j,i} G^*)_{l,k} L(E_{i,j})_{k,l} \\
&= \sum_{k \in J} \sum_{i,j \in J} \sum_{l \in J} (G E_{i,j} F^*)_{l,k}^* L(E_{i,j})_{k,l}.
\end{aligned}$$

In these equations we used that $\langle x \otimes y, v \otimes w \rangle = \langle x, v \rangle \langle y, w \rangle$. Furthermore, because this is the product of Hilbert-Schmidt operators, these sums are absolutely convergent. Hence, we can interchange summations yielding

$$\sum_{k \in J} \sum_{i,j \in J} \sum_{l \in J} (G E_{i,j} F^*)_{l,k}^* L(E_{i,j})_{k,l} = \text{Tr} \left(\sum_{i,j \in J} (G E_{i,j} F^*)^* L(E_{i,j}) \right) \quad (4.33)$$

$$= \langle (\#G \otimes F^*), L \rangle_{\mathcal{L}_2(\mathcal{H}')} \quad (4.34)$$

This completes the proof. ■

Notice that leaving out the identity of $\mathcal{L}_4(\mathcal{L}_3(\mathcal{H}))$ is not a problem, since the operators of interest have $LI = 0$, which the identity is surely not. Furthermore, the operators $L \in \mathcal{L}_2(\mathcal{L}_2(\mathcal{H})')$ are not defined on the identity. Recall that for L to generate a norm continuous semigroup we require L to be ultraweakly continuous. This in combination with $LI = 0$ yields that this extension is still CP, which follows from the fact that a sequence $0 \leq X_n$ (for instance n ones on the diagonal) with $X_n \rightarrow I$ ultraweakly and $X_n \rightarrow I$ weakly, implies that $LX_n \rightarrow LI = 0$ ultraweakly. Furthermore, if we have a matrix $(X_{i,j}) \in M_k(\mathcal{L}_2(\mathcal{H})')$ with one (or more) entry(ies) being X_n , then for increasing $n \in \mathbb{N}$ $L(X_n)$ gets closer and closer to LI . Since $L((X_{i,j}))$ is positive for all $n \in \mathbb{N}$, we must have that it is positive for the entry X_n replaced by I . Hence, the extension of L to I is CP by the requirement that L is ultraweakly continuous on $\mathcal{L}_3(\mathcal{H})$, which we always assume to make the generated semigroup norm continuous.

By lemma 4.18 we know that by studying the GKS matrix of an operator L we obtain information about L , one of the properties of interest is the complete positivity of L . The theorem of the Choi matrix states, in the finite dimensional case, that an operator is CP if and only if its Choi matrix is positive. Furthermore, a positive Choi matrix if and only if an operator is CP is even more general; Friedland [10] proved that this fact can be generalised to countable infinite dimensions. Unfortunately, this does require a stronger assumption on L . Namely, L should map strongly convergent sequences to weakly convergent sequences. I.e. suppose $(X_n)_{n \in \mathbb{N}} \subset B(\mathcal{H})$ and $L : B(\mathcal{H}) \rightarrow B(\mathcal{H})$, then if $X_n \rightarrow X$ in the SOT, we must have $LX_n \rightarrow LX$ in the WOT, from now on we will call this assumption STW (strong to weak). Under this assumption Choi's theorem can be generalised to countable infinite dimensions (theorem 4 in Friedland [10]). To state:

Theorem 4.19. Let \mathcal{H} be a Hilbert space with a countable infinite basis $(e_n)_{n \in \mathbb{N}}$ and set $E_{i,j} = e_i e_j^*$. Furthermore, denote P_m the projection of \mathcal{H} on $\text{span}(e_1, e_2, \dots, e_m)$ for all $m \in \mathbb{N}$. Assume that $L : B(\mathcal{H}) \rightarrow B(\mathcal{H})$ is a bounded linear operator which maps sequences converging in the SOT to sequences converging in the WOT, i.e. L is STW. Then L is CP if and only if for each $n \in \mathbb{N}$ the matrix $\mathcal{C}(L) = (P_n L(E_{i,j}) P_n)_{i,j=0}^n$ is positive.

Hence, a positive Choi matrix leads to a CP operator. Additionally, lemma 4.18 proves the equivalence of the Choi matrix and the GKS matrix. Therefore, we can study the GKS matrix and obtain information about the complete positivity of operators.

4.2.2. THE LINDBLAD FORM FOR TRACE CLASS OPERATORS

This section considers the derivation of the Lindblad form for the trace class operators with a Hilbert-Schmidt inner product and shows that these types of operators are actually generators of Quantum Markov Semigroups (QMS).

We know by proposition 4.12 that the considered operators preserve $\mathcal{L}_3(\mathcal{H})$. Furthermore, it is useful to split the GKS matrix into two parts. To this end, we will label our basis with a double index. I.e. let $\{F_\mu\}$ be an orthonormal basis, with $\mu \in J \times J$, where J is again a countable index set. Using this basis we define the reduced GKS matrix as follows.

Definition 4.20. Let $L \in \mathcal{L}_4(\mathcal{L}_3(\mathcal{H}))$ such that L is self-adjoint, L is STW, $LI = 0$ and $LX^* = (LX)^*$ for all $X \in \mathcal{L}_3(\mathcal{H})$. We now pick an orthonormal basis $\{F_\mu\}$ of $\mathcal{L}_3(\mathcal{H})$, where we set $F_{(1,1)}$ equal to the identity. Furthermore, we set $c_{\alpha,\beta}$ to be the GKS matrix of L with respect to the

$\{F_\mu\}$ basis. Then the reduced GKS matrix is defined to be the matrix $c_{\alpha,\beta}$, where $\alpha, \beta \in A$ and $A = \{(i, j) : i, j \in J \text{ and } (i, j) \neq (1, 1)\}$.

The reason we are defining this quantity is because ideally we would like to remove any dependence of our operator on I , because we would much rather work with just $\mathcal{L}_2(\mathcal{L}_2(\mathcal{H}))$ instead of $\mathcal{L}_4(\mathcal{L}_3(\mathcal{H}))$. The reduced GKS matrix is therefore a perfect tool to use, because we only consider the projection of L onto the space $\mathcal{L}_2(\mathcal{H})'$. Additionally, for the requirements stated $L \neq I$. Hence, the space of operators is reduced to the Hilbert-Schmidt operators. Furthermore, we would like to show that we can use the reduced GKS matrix of L to know whether the semigroups generated by L are CP. To this end we introduce the following lemma.

Lemma 4.21. Let $L \in \mathcal{L}_4(\mathcal{L}_3(\mathcal{H}))$ with L STW, L self-adjoint, $LI = 0$ and $LX^* = (LX)^*$ and set $\Phi_t = e^{tL}$. Let $\{F_\mu\}$ be an orthonormal basis of $\mathcal{L}_3(\mathcal{H})$, with $F_{(1,1)} = I$. Let $c_{\alpha,\beta}$ be the GKS matrix of L with respect to $\{F_\mu\}$. Then $\Phi_t \in \text{CP}(\mathcal{L}_3(\mathcal{H}))$ for $t \geq 0$ if and only if the reduced GKS matrix of L is positive.

Proof. We begin with proving the forward implication. Hence, suppose first that Φ_t as defined is completely positive for $t \geq 0$. We will use the definition of a generator as defined in 1.31, then

$$c_{\alpha,\beta}(L) = \lim_{t \rightarrow \infty} c_{\alpha,\beta} \left(\frac{\Phi_t - I}{t} \right) = \lim_{t \rightarrow \infty} \left(\frac{c_{\alpha,\beta}(\Phi_t)}{t} - \frac{c_{\alpha,\beta}(I)}{t} \right). \quad (4.35)$$

Interchanging the limit and $c_{\alpha,\beta}$ is allowed by the fact that $\Phi_t - I \in \mathcal{L}_4(\mathcal{L}_3(\mathcal{H}))$, which follows from

$$\Phi_t - I = I + tL + \dots + \frac{(tL)^n}{n!} + \dots - I = tL + \dots + \frac{(tL)^n}{n!} + \dots \in \mathcal{L}_4(\mathcal{L}_3(\mathcal{H})). \quad (4.36)$$

Where we know that the last expression is in $\mathcal{L}_4(\mathcal{L}_3(\mathcal{H}))$ by the fact that $L \in \mathcal{L}_4(\mathcal{L}_3(\mathcal{H}))$. Additionally, we can split up the $c_{\alpha,\beta}$ of $\Phi_t - I$ due to the fact that both Φ_t and I are in $\mathcal{L}_4(\mathcal{L}_3(\mathcal{H}))$ by construction of $\mathcal{L}_4(\mathcal{L}_3(\mathcal{H}))$. Furthermore, we know that $c_{\alpha,\beta}(I) \neq 0$ only if $\alpha = (1, 1)$ and $\beta = (1, 1)$ due to the orthonormal "basis" or set we used to construct the GKS matrix. Therefore, only considering the reduced GKS matrix of L is equivalent to only considering the reduced GKS of $\frac{\Phi_t}{t}$. In particular, we need this to be positive to prove the claim. However, due to lemma 4.18 we know that a CP operator has a positive GKS matrix. Hence, we can conclude that the reduced GKS matrix of L is positive.

To prove the backward implication, suppose the reduced GKS matrix of L is positive. Then we can expand the GSK matrix of every semigroup as

$$c_{\alpha,\beta}(\Phi_t) = c_{\alpha,\beta}(I) + tc_{\alpha,\beta}(L) + \mathcal{O}(t^2). \quad (4.37)$$

For sufficiently small $t \geq 0$ the reduced GKS matrix is positive, since $c_{\alpha,\beta}(I) = 0$. Hence, since the reduced GKS is positive, Φ_t is in CP. By the semigroup property of multiplication, Φ_t is CP for all $t \geq 0$, since $\Phi_t \Phi_t = \Phi_{2t}$. ■

Now that we know that our formalism works in describing Quantum Markov Semigroups, we want to start simplifying the Lindblad equation for a generator L . However, we first need to obtain a general form that incorporates the reduced GKS matrix. Therefore, we prove the following proposition.

Proposition 4.22. Let $L \in \mathcal{L}_4(\mathcal{L}_3(\mathcal{H}))$ such that L is self-adjoint, L is STW, $LI = 0$ and $(LX)^* = LX^*$ for all $X \in \mathcal{L}_3(\mathcal{H})$. Let $\{F_\mu\}$ be an orthonormal basis of $\mathcal{L}_3(\mathcal{H})$ such that $F_{(1,1)} = I$. Let $c_{\alpha,\beta}$ be the GKS matrix of L with respect to $\{F_\mu\}$. Then L is given by

$$LX = \frac{1}{2} \sum_{\alpha,\beta \neq (1,1)} c_{\alpha,\beta} (F_\alpha^* [X, F_\beta] + [F_\alpha^*, X] F_\beta). \quad (4.38)$$

Notice that the summation sums over all entries except the indices associated with the identity I . Hence, the matrix in the summation is the reduced GKS matrix of L .

Proof. It should be noted that $c_{(1,1),\beta}$ and $c_{\beta,(1,1)}$ for $\beta \in J$ are all 0. This can be seen by applying the self-adjointness of L and the fact that $LI = 0$, which yields

$$\begin{aligned} c_{(1,1),\beta} &= \left\langle \# \left(F_{(1,1)}^* \otimes F_\beta \right), L \right\rangle_{\mathcal{L}_4(\mathcal{L}_3(\mathcal{H}))} \\ &= \text{Tr} \left(F_{(1,1)} L F_\beta^* \right) \\ &= \text{Tr} \left(L(I) F_\beta^* \right) \\ &= 0. \end{aligned}$$

Notice that if $\beta = (1,1)$ the first equation would immediately be zero by construction, this is also the case in the next part. Similarly, we can write

$$\begin{aligned} c_{\beta,(1,1)} &= \left\langle \# \left(F_\beta^* \otimes F_{(1,1)} \right), L \right\rangle_{\mathcal{L}_4(\mathcal{L}_3(\mathcal{H}))} \\ &= \text{Tr} \left(F_\beta L F_{(1,1)}^* \right) \\ &= 0. \end{aligned}$$

This fact allows us to split up the normal GKS decomposition. Hence, by applying lemma 4.16 we know that $c_{\alpha,\beta}$ is self-adjoint. Therefore, we can write for all $X \in \mathcal{L}_3(\mathcal{H})$

$$LX = \sum_{\alpha,\beta} c_{\alpha,\beta} F_\alpha^* X F_\beta = G^* X + XG + \sum_{\alpha,\beta \neq (1,1)} c_{\alpha,\beta} F_\alpha^* X F_\beta. \quad (4.39)$$

Where we defined $G = \sum_{\beta} c_{(1,1),\beta} F_\beta$. Furthermore, we can decompose $G = K + iH$, where both K and H are both self-adjoint, since they are both 0. Hence,

$$LX = -i[H, X] + KA + AK + \sum_{\alpha,\beta \neq (1,1)} c_{\alpha,\beta} F_\alpha^* X F_\beta. \quad (4.40)$$

Which for the case $X = I$ simplifies to

$$LI = 2K + \sum_{\alpha,\beta \neq (1,1)} c_{\alpha,\beta} F_\alpha^* F_\beta = 0. \quad (4.41)$$

Thus $K = -\frac{1}{2} \sum_{\alpha,\beta \neq (1,1)} c_{\alpha,\beta} F_\alpha^* F_\beta$, which immediately implies that

$$LX = -i[H, X] + KA + AK + \sum_{\alpha,\beta \neq (1,1)} c_{\alpha,\beta} F_\alpha^* X F_\beta = \frac{1}{2} \sum_{\alpha,\beta \neq (1,1)} c_{\alpha,\beta} (F_\alpha^* [X, F_\beta] + [F_\alpha^*, X] F_\beta), \quad (4.42)$$

In the last equation we used the fact that $G = 0$, which implies that both K and H have to be zero, thus the commutator drops out and we have the result as required. \blacksquare

4.3. MODULAR AUTOMORPHISMS GROUP

This section covers the modular automorphisms group, which describes time translation along a particular Hamiltonian. We begin with its definition and certain properties. Additionally, we define a new inner product. Furthermore, if a generator is self-adjoint with respect to this inner product it commutes with the modular automorphisms group. Hence, the associated QMS $\Phi_t = e^{tL}$ is time invariant. This is the extra structure we want to apply to our generator to derive a new and simplified version of the Lindblad equation. Lastly, we prove a theorem that shows the special commutation of the GKS matrix with the eigenvalues of the modular operator.

To study the symmetry that we actually want to obtain, we start of by defining the modular automorphisms group. However, we will first introduce some useful notation.

Notation 4.23. The invertible density operators of $\mathcal{L}_3(\mathcal{H})$ are denoted \mathfrak{S}_+ .

Definition 4.24. Let $\sigma \in \mathfrak{S}_+$. We define Δ_σ , also called the modular operator, to be the linear operator on $\mathcal{L}_3(\mathcal{H})$ that works on $X \in \mathcal{L}_3(\mathcal{H})$ as

$$\Delta_\sigma(X) = \sigma X \sigma^{-1}. \quad (4.43)$$

Furthermore, the modular generator is defined to be the self-adjoint element in $\mathcal{L}_3(\mathcal{H})$ by functional calculus of the logarithm as

$$h = -\log(\sigma). \quad (4.44)$$

Lastly, the modular automorphism group α_t on $\mathcal{L}_3(\mathcal{H})$ is the group defined as

$$\alpha_t(X) = e^{ith} X e^{-ith}, \quad (4.45)$$

for $t \in \mathbb{C}$ and e^{ith} given by the operator exponential.

If we look carefully at equation 4.45 we see that this resembles unitary evolution of an operator X in the Heisenberg picture with Hamiltonian h . However, we are interested in the operator Δ_σ , which is the same as the modular automorphism group if $t = i$, which is not a physical time. However, multiple results that we derive in this section apply to α_t in general and hence have a physical concept behind them.

Now that we have defined the modular operator, we can notice that it is positive and self-adjoint with respect to the Hilbert-Schmidt inner product. Indeed, for all $X, Y \in \mathcal{L}_3(\mathcal{H})$ with $X, Y \neq I$ we have

$$\langle X, \Delta_\sigma Y \rangle = \text{Tr}(X^* \Delta_\sigma Y) = \text{Tr}(\sigma^{-1} X^* \sigma Y) = \text{Tr}(\Delta_\sigma^{-1} X^* Y) = \text{Tr}((\Delta_\sigma X)^* Y) = \langle \Delta_\sigma X, Y \rangle, \quad (4.46)$$

and

$$\text{Tr}(X^* \Delta_\sigma X) = \text{Tr}\left(|\sigma^{1/2} X \sigma^{-1/2}|^2\right). \quad (4.47)$$

For the identity cases we need different cases, but it is less work

$$\langle I, \Delta_\sigma Y \rangle = 0 = \langle \Delta_\sigma I, Y \rangle = \langle I, Y \rangle, \quad (4.48)$$

$$\langle X, \Delta_\sigma I \rangle = \langle X, I \rangle = 0 = \langle \Delta_\sigma X, I \rangle, \quad (4.49)$$

$$\langle I, \Delta_\sigma I \rangle = \langle I, I \rangle = 1 = \langle \Delta_\sigma I, I \rangle, \quad (4.50)$$

and for the positivity we can see that this is true by the values that the inner product takes in the different cases. Furthermore, the fact that Δ_σ is a positive self-adjoint operator implies that there exists an orthonormal basis of eigenoperators of Δ_σ with strictly positive eigenvalues. These can be written as e^ω since the exponential function is a continuous, surjective function on the positive real numbers. Furthermore, we have $\Delta_\sigma(I) = I$. Moreover, $\Delta_\sigma^{-1}X^* = (\Delta_\sigma X)^*$, which implies that if X is an eigenvector of Δ_σ with eigenvalue $e^{-\omega}$ then X^* is an eigenvector with eigenvalue e^ω . Hence, we can state the following.

Definition 4.25. Let $\sigma \in \mathfrak{S}_+$ be a density operator. Then there exists an orthonormal basis called the modular basis of $\mathcal{L}_3(\mathcal{H})$ with the following properties:

1. $\{F_1, \dots\}$ consists of eigenvectors of Δ_σ .
2. $F_1 = I$.
3. $\{F_1, \dots\} = \{F_1^*, \dots\}$, i.e. if F_i is a eigenvector then F_i^* is also an eigenvector by the previous discussion.

Aside from the eigenbasis of Δ_σ we require an additional inner product, parameterized by a parameter $s \in [0, 1]$.

Definition 4.26. Let $\sigma \in \mathfrak{S}_+$ a density operator, which is non degenerate. For all $X, Y \in \mathcal{L}_3(\mathcal{H})$, define

$$\langle X, Y \rangle_s = \text{Tr}\left(\left(\sigma^{(1-s)/2} X \sigma^{s/2}\right)^* \left(\sigma^{(1-s)/2} Y \sigma^{s/2}\right)\right) = \text{Tr}(\sigma^s X^* \sigma^{1-s} Y). \quad (4.51)$$

This inner product allows us to specify the symmetry that will simplify the Lindblad equation. Before we can state the symmetry theorem, we require the following lemma.

Lemma 4.27. For all $X, Y \in \mathcal{L}_3(\mathcal{H})$ we have,

$$\langle \alpha_{it} X, Y \rangle_s = \langle X, Y \rangle_{s-t} = \langle X, \alpha_{it} B \rangle_s. \quad (4.52)$$

The proof is fortunately very straightforward.

Proof.

$$\begin{aligned} \langle \alpha_{it} X, Y \rangle_s &= \text{Tr}(\sigma^s (\sigma^t X \sigma^{-t})^* \sigma^{1-s} Y) \\ &= \text{Tr}(\sigma^{s-t} X^* \sigma^{1-s+t} Y) \\ &= \langle X, Y \rangle_{s-t} \\ &= \text{Tr}(\sigma^s X^* \sigma^{1-s} (\sigma^t Y \sigma^{-t})) \\ &= \langle X, \alpha_{it} Y \rangle. \end{aligned}$$

■

Hence, α_{it} is self-adjoint with respect to the inner product. Furthermore, this lemma is important in proving the next theorem.

Theorem 4.28. Let $\sigma \in \mathfrak{S}_+$ be a non-degenerate density operator and let $s \in [0, 1]$, $s \neq \frac{1}{2}$. Let $L \in \mathcal{L}_4(\mathcal{L}_3(\mathcal{H}))$ such that $LX^* = (LX)^*$ for all $X \in \mathcal{L}_3(\mathcal{H})$. Furthermore, assume that L is self-adjoint with respect to $\langle \cdot, \cdot \rangle_s$. Then L commutes with α_t for all $t \in \mathbb{C}$.

It should be noted that $s = 1/2$ is a special case for which the inner product $\langle \cdot, \cdot \rangle_{1/2}$ is called the KMS inner product. We will not dive into the meaning and reasons why this is a special case. However, for the interested reader we recommend Carlen and Maas [6] Appendix B and for states associated with the KMS inner product one can read Brattelli and Robinson [4] (pages 76-144).

Proof. Let $X, Y \in \mathcal{L}_3(\mathcal{H})$. Then

$$\begin{aligned}
\langle L\alpha_{i(2s-1)}(X), Y \rangle_s &= \text{Tr}(\sigma^s(L(\sigma^{2s-1}X\sigma^{1-2s}))^* \sigma^{1-s}Y) \\
&= \text{Tr}(\sigma^s(\sigma^{2s-1}X\sigma^{1-2s})^* \sigma^{1-s}L(Y)) && L \text{ is self-adjoint in } \langle \cdot, \cdot \rangle_s \\
&= \text{Tr}(\sigma^s \sigma^{1-2s} X^* \sigma^{2s-1} \sigma^{1-s} L(Y)) \\
&= \text{Tr}(\sigma^s L(Y) \sigma^{1-s} X^*) && \text{Trace cyclicity} \\
&= \text{Tr}(\sigma^s (L(Y^*))^* \sigma^{1-s} X^*) && LY^* = (LY)^* \\
&= \text{Tr}(\sigma^s Y \sigma^{1-s} L(X^*)) && L \text{ is self-adjoint in } \langle \cdot, \cdot \rangle_s \\
&= \text{Tr}(\sigma^s Y \sigma^{1-s} (LX)^*) && LY^* = (LY)^* \\
&= \text{Tr}(\sigma^{1-s} (LX)^* \sigma^s Y) && \text{Trace cyclicity} \\
&= \langle L(X), Y \rangle_{1-s}.
\end{aligned}$$

In these equations the cyclicity is again justified by the fact that products of Hilbert-Schmidt operators are Hilbert-Schmidt. Furthermore, notice that by applying lemma 4.27 we obtain

$$\langle L(X), Y \rangle_{1-s} = \langle L(X), Y \rangle_{s-2s-1} = \langle \alpha_{it}(LX), Y \rangle_s. \quad (4.53)$$

Hence, by this logic we have $\langle L\alpha_{it}(X), Y \rangle_s = \langle \alpha_{it}(LX), Y \rangle_s$. By the fact that both X and Y were arbitrary we have that $\alpha_{i(2s-1)}L = L\alpha_{i(2s-1)}$. Hence, L commutes with $\alpha_{i(2s-1)}$, in particular it commutes with every polynomial in $\alpha_{i(2s-1)}$. Therefore it commutes with every continuous function in $\alpha_{i(2s-1)}$. Specifically, this fact yields that L commutes with α_t for all t . ■

We now know that self-adjointness of L with respect to $\langle \cdot, \cdot \rangle_s$ along with our other assumptions on L leads to it commuting with time translation along a Hamiltonian. Furthermore, Alicki [1] concluded that every QMS $\Phi_t = e^{tL}$ has $L(X^*) = (LX)^*$ and thus $\Phi_t(X^*) = (\Phi_t X)^*$. Hence, if Φ_t is self-adjoint with respect to $\langle \cdot, \cdot \rangle_1$ for some $\sigma \in \mathfrak{S}_+$ a density operator, we have that

$$\Phi_t(\alpha_{t'}X) = \alpha_{t'}\Phi_t(X) \quad \text{for all } X \in \mathcal{L}_3(\mathcal{H}) \text{ and for all } t \geq 0, t' \in \mathbb{C}. \quad (4.54)$$

Therefore, we have time invariance for Φ_t . Notice that in our discussion we set $s = 1$, which is a special case called the GNS or Gelfand-Naimark-Segal inner product. This inner product is closely related to the expectation value of an operator, i.e. $\text{Tr}(\sigma X^* Y) = \langle X^* Y \rangle$ as discussed in chapter 1.

To state the main theorem of this section, we first need to explicitly construct a proper modular basis with indices $\mu = (\mu_1, \mu_2)$ and their eigenvalues. To this end, consider the modular generator $h = -\log \sigma$ for some density operator $\sigma \in \mathfrak{S}_+$. Then let $\{x_1, x_2, \dots\}$ be an infinite countable basis of \mathcal{H} consisting of eigenvectors of h and set λ_i to be the eigenvalue of eigenvector x_i . We define $F_\mu = F_{(\mu_1, \mu_2)} = x_{\mu_1} x_{\mu_2}^*$, which is similar to our previous $E_{i,j}$ only now we are not considering the standard basis of \mathcal{H} . Furthermore, since $\sigma = e^{-h}$ we then obtain that

$$\Delta_\sigma F_\mu = e^{\mu_2 - \mu_1} F_\mu = e^{-\omega_\mu} F_\mu. \quad (4.55)$$

It is clear that $F_\mu^* = F_{\mu'}$ with $\mu' = (\mu_2, \mu_1)$. Consider $\{F_\mu\}$, we see that, by setting $F_{(1,1)} = I$ and taking into consideration the previous comment, this is a modular basis of $\mathcal{L}_3(\mathcal{H})$.

Having constructed a modular basis, we can now exploit time invariance of a self-adjoint QMS with respect to $\langle \cdot, \cdot \rangle_s$ for some $\sigma \in \mathfrak{S}_+$ a density matrix, to state the following theorem, which is the main result of this section.

Theorem 4.29. Let $L \in \mathcal{L}_4(\mathcal{L}_3(\mathcal{H}))$ self-adjoint be the generator of a QMS on $\mathcal{L}_3(\mathcal{H})$ that is self-adjoint with respect to the inner product $\langle \cdot, \cdot \rangle_s$ for $s \in [0, 1]$ and $s \neq 1/2$ and for some $\sigma \in \mathfrak{S}_+$ a density operator. Let $\{F_\mu\}$ be the modular basis of Δ_σ as previously constructed. Additionally, let $c_{\alpha,\beta}$ be the GKS matrix of L with respect to $\{F_\mu\}$. Then for all α, β we have that

$$e^{\omega_\alpha} c_{\alpha,\beta} = c_{\alpha,\beta} e^{\omega_\beta}, \quad (4.56)$$

and

$$c_{\alpha,\beta} = e^{-\omega_\alpha} c_{\alpha',\beta'}. \quad (4.57)$$

In this equation the ω_α are as defined in equation 4.55.

Proof. By the fact that L is a generator of a QMS, we have $LX^* = (LX)^*$ for all $X \in \mathcal{L}_3(\mathcal{H})$. Additionally, $LI = 0$. Furthermore, by theorem 4.28 we have that L commutes with the modular automorphisms group. Therefore, for all $X \in \mathcal{L}_3(\mathcal{H})$ we can apply this fact, the GKS expansion and equation 4.55 to obtain

$$LX = \sigma^{-1}(L(\sigma X \sigma^{-1}))\sigma = \sum_{\alpha,\beta} c_{\alpha,\beta} \sigma^{-1} F_\alpha^* \sigma X \sigma^{-1} F_\beta \sigma = \sum_{\alpha,\beta} c_{\alpha,\beta} e^{\omega_\beta - \omega_\alpha} F_\alpha^* X F_\beta. \quad (4.58)$$

This equation implies

$$\sum_{\alpha,\beta} c_{\alpha,\beta} e^{\omega_\beta - \omega_\alpha} F_\alpha^* X F_\beta = \sum_{\alpha,\beta} c_{\alpha,\beta} F_\alpha^* X F_\beta. \quad (4.59)$$

Since, the coefficients of the GKS expansion are unique, we now see $c_{\alpha,\beta} e^{\omega_\beta} = e^{\omega_\alpha} c_{\alpha,\beta}$. Hence, we move on to the second claim.

First, we will derive a GKS decomposition for the adjoint. To this end, let $X, Y \in \mathcal{L}_3(\mathcal{H})$, then the product $(LX)^* Y$ Hilbert-Schmidt, therefore the sum of coefficients converges absolutely and allows us to take out the sum of the trace in a similar way to the proof of lemma 4.14.

$$\begin{aligned} \langle LX, Y \rangle &= \text{Tr}((LX)^* Y) \\ &= \sum_{\alpha,\beta} \text{Tr}\left(\overline{c_{\alpha,\beta}} F_\beta^* X^* F_\alpha Y\right) \\ &= \sum_{\alpha,\beta} \text{Tr}\left(X^* \overline{c_{\alpha,\beta}} F_\alpha Y F_\beta^*\right) = \langle X, L^* Y \rangle. \end{aligned}$$

By lemma 4.16 we know that $\overline{c_{\alpha,\beta}} = c_{\beta,\alpha}$. Hence, $L^* X = \sum_{\alpha,\beta} c_{\beta,\alpha} F_\alpha X F_\beta^*$. Furthermore, we can now compute what the adjoint of L would be in the $\langle \cdot, \cdot \rangle_s$ inner product. Hence,

$$\begin{aligned} \langle LX, Y \rangle_s &= \text{Tr}((LX)^* \sigma^{1-s} Y \sigma^s) \\ &= \text{Tr}(X^* L^* (\sigma^{1-s} Y \sigma^s)) \\ &= \langle X, \sigma^{1-s} L^* (\sigma^{1-s} Y \sigma^s) \sigma^{-s} \rangle_s. \end{aligned}$$

Hence, we obtain $L^*Y = \sigma^{1-s}L^*(\sigma^{1-s}Y\sigma^s)\sigma^{-s} = LY$, where the last equality follows from the fact that L is self-adjoint with respect to $\langle \cdot, \cdot \rangle_s$. Thus, by combining our two previous results we obtain

$$\begin{aligned}
LX &= \sum_{\alpha, \beta} c_{\alpha, \beta} F_{\alpha}^* X F_{\beta} \\
&= \sigma^{1-s} L^* (\sigma^{1-s} Y \sigma^s) \sigma^{-s} \\
&= \sum_{\alpha, \beta} c_{\beta, \alpha} \sigma^{1-s} F_{\alpha} \sigma^{1-s} Y \sigma^s F_{\beta}^* \sigma^{-s} \\
&= \sum_{\alpha, \beta} c_{\beta, \alpha} \Delta_{\sigma}^{1-s} F_{\alpha} Y \Delta_{\sigma}^s F_{\beta}^* \\
&= \sum_{\alpha, \beta} c_{\beta, \alpha} e^{(1-s)\omega_{\alpha}} e^{s\omega_{\beta}} F_{\alpha} Y F_{\beta}^*.
\end{aligned}$$

The modular basis has that if F_{μ} is a basisvector with eigenvalue ω_{μ} then $F_{\mu'} = F_{\mu}^*$ is a basisvector, with eigenvalue $\omega_{\mu'} = -\omega_{\mu}$. Hence,

$$\sum_{\alpha, \beta} c_{\beta, \alpha} e^{(1-s)\omega_{\alpha}} e^{s\omega_{\beta}} F_{\alpha} Y F_{\beta}^* = \sum_{\alpha, \beta} c_{\beta, \alpha} e^{(s-1)\omega_{\alpha'}} e^{s\omega_{\beta'}} F_{\alpha'}^* X F_{\beta'}. \quad (4.60)$$

Now, we can re-index by $\alpha' \leftrightarrow \alpha$ and $\beta' \leftrightarrow \beta$, to obtain

$$\sum_{\alpha, \beta} c_{\alpha, \beta} F_{\alpha}^* X F_{\beta} = \sum_{\alpha, \beta} c_{\beta', \alpha'} e^{(s-1)\omega_{\alpha}} e^{s\omega_{\beta}} F_{\alpha}^* X F_{\beta}. \quad (4.61)$$

Since the identity in equation 4.56 implies that $c_{\alpha, \beta}$ commutes with powers of $e^{\omega_{\alpha}}$ in a particular fashion and by applying the fact that the GKS coefficients are unique, it follows that

$$e^{(1-s)\omega_{\alpha}} c_{\alpha, \beta} e^{s\omega_{\beta}} = e^{\omega_{\alpha}} c_{\alpha, \beta} = c_{\beta', \alpha'}. \quad (4.62)$$

Which completes the proof. ■

These two relations for the GKS matrix are helpful in proving the main result of this dissertation, which is considered in the next section.

4.4. THE MAIN RESULT

This section contains the main result of this dissertation, the Lindblad form for generators that are self-adjoint with respect to the GNS inner product for some density operator $\sigma \in \mathfrak{S}_+$, for \mathcal{H} a countable infinite dimensional Hilbert space. These generators have a Lindblad form, which is greatly simplified in contrast to the general Lindblad form, which is shown in theorem 4.30.

The main result of this dissertation is as follows.

Theorem 4.30. Let $\Phi_t = e^{tL}$ be a QMS on $\mathcal{L}_3(\mathcal{H})$, with $L \in \mathcal{L}_4(\mathcal{L}_3(\mathcal{H}))$ self-adjoint and L STW. Suppose that Φ_t is self-adjoint with respect to the GNS inner product for some $\sigma \in \mathfrak{S}_+$ a den-

sity operator. Then for all $X \in \mathcal{L}_3(\mathcal{H})$ the generator L of Φ_t is of the form

$$LX = \sum_{j \in J} \left(e^{-\omega_j/2} V_j^* [X, V_j] + e^{\omega_j/2} [V_j, X] V_j^* \right) \quad (4.63)$$

$$= \sum_{j \in J} e^{-\omega_j/2} \left(V_j^* [X, V_j] + [V_j^*, X] V_j \right) \quad (4.64)$$

with $\omega_j \in \mathbb{R}$ for all $j \in J$ and $\{V_j\}_{j \in J}$ is a modular basis with the identity element removed, i.e. $V_1 = I \notin \{V_j\}_{j \in J}$. Conversely, if $L \in \mathcal{L}_4(\mathcal{L}_3(\mathcal{H}))$ is a self-adjoint and STW generator expressed in a set $\{V_j\}_{j \in J}$ that has the properties of a modular basis without the identity. Then L generates a QMS that is self-adjoint with respect to the GNS inner product for some $\sigma \in \mathfrak{S}_+$ a density operator.

Proof. First set $\{F_\mu\}$ to be a modular basis of $\mathcal{L}_3(\mathcal{H})$ with respect to σ , we require that the reduced GKS matrix is diagonal with respect to this basis. We are allowed to do this from the fact that the GKS matrix is self-adjoint by lemma 4.16. Notice that by applying proposition 4.22 we can decompose L for all $X \in \mathcal{L}_3(\mathcal{H})$ as follows

$$LX = \frac{1}{2} \sum_{\alpha, \beta \neq (1,1)} c_{\alpha, \beta} (F_\alpha^* [X, F_\beta] + [F_\alpha^*, X] F_\beta). \quad (4.65)$$

This is the first part of the Lindblad equation. Next consider the general GKS form and the fact that $F_{\mu'} = F_\mu^*$, which yields

$$\begin{aligned} LX &= \sum_{\alpha, \beta} c_{\alpha, \beta} F_\alpha^* X F_\beta = \sum_{\alpha, \beta} c_{\alpha, \beta} F_{\alpha'} X F_{\beta'}^* \\ &= \sum_{\alpha, \beta} c_{\beta', \alpha'} F_\beta X F_\alpha^* \\ &= \sum_{\alpha, \beta} c_{\alpha, \beta} e^{\omega_\alpha} F_\beta X F_\alpha^*. \end{aligned}$$

In the second to last inequality, we re-indexed by $\alpha \leftrightarrow \beta'$ and $\beta \leftrightarrow \alpha'$. Furthermore, in the last equality we invoked theorem 4.29 to write $c_{\beta', \alpha'} = c_{\alpha, \beta} e^{\omega_\alpha}$. By applying proposition 4.22 again we can write

$$LX = \frac{1}{2} \sum_{\alpha, \beta \neq (1,1)} c_{\alpha, \beta} e^{\omega_\alpha} (F_\beta [X, F_\alpha^*] + [F_\beta, X] F_\alpha^*). \quad (4.66)$$

By taking the average over both expressions of L we obtain

$$LX = \frac{1}{4} \sum_{\alpha, \beta \neq (1,1)} c_{\alpha, \beta} [(F_\alpha^* [X, F_\beta] + [F_\alpha^*, X] F_\beta) + e^{\omega_\alpha} (F_\beta [X, F_\alpha^*] + [F_\beta, X] F_\alpha^*)]. \quad (4.67)$$

By applying the fact that the reduced GKS matrix of L is diagonal with respect to the modular basis we obtain a diagonal form, written as

$$c_{\alpha, \beta} = \sum_{\gamma \neq (1,1)} \delta_{\alpha, \gamma} \delta_{\beta, \gamma} d_\gamma = 2 \sum_{\gamma \neq (1,1)} \delta_{\alpha, \gamma} \delta_{\beta, \gamma} c_\gamma e^{-\omega_\gamma/2}. \quad (4.68)$$

In the last equation we simply re-scaled the diagonal form constant. Applying this decomposition yields the following expression

$$LX = \frac{1}{2} \sum_{\gamma \neq (1,1)} c_\gamma \left[e^{-\omega_\gamma/2} \left(F_\gamma^* [X, F_\gamma] + [F_\gamma^*, X] F_\gamma \right) + e^{\omega_\gamma/2} \left(F_\gamma [X, F_\gamma^*] + [F_\gamma, X] F_\gamma^* \right) \right]. \quad (4.69)$$

Now by symmetry we can assume that $c_\gamma = c_{\gamma'}$, such that $V_{\gamma'} = V_\gamma^*$, where we have set $V_\gamma = F_\gamma$. Which then yields,

$$LX = \sum_{\gamma \neq (1,1)} c_\gamma \left[e^{-\omega_\gamma/2} V_\gamma^* [X, V_\gamma] + e^{\omega_\gamma/2} [V_\gamma, X] V_\gamma^* \right]. \quad (4.70)$$

If we use the diagonalization immediately in equation 4.65 we obtain the other form.

$$LX = \sum_{\gamma \neq (1,1)} c_\gamma e^{-\omega_\gamma/2} \left(V_\gamma^* [X, V_\gamma] + [V_\gamma^*, X] V_\gamma \right). \quad (4.71)$$

We can now set $V_\gamma \rightarrow \sqrt{c_\gamma} V_\gamma$ by the fact that the reduced GKS matrix is positive, therefore all c_γ are positive and thus the square root exists. Now take $J = \{\gamma : \gamma \neq (1, 1)\}$ and we are done. For the converse, assume that L has the specified form. We can take out the c_γ by applying the normalization and making all V_γ into an orthonormal basis, adding in the V_γ with $c_\gamma = 0$ and the identity. Furthermore, it is obvious that $LI = 0$ from the decomposition and therefore by lemma 4.21 L generates a QMS. Additionally, since the V_γ are eigenvectors of Δ_σ , it follows that the semigroup commutes with Δ_σ . Now let $X, Y \in \mathcal{L}_3(\mathcal{H})$ with $X, Y \neq I$ (in this case the next expression would be 0) and notice the fact that X, Y and L are all Hilbert Schmidt operators, thus by the same argument we used many times before: the trace converges absolutely, allowing us to interchange the summations. We then have

$$\begin{aligned} \langle X, LY \rangle_{1/2} &= \text{Tr}(\Delta_\sigma^{1/2}(X^*)LY) \\ &= \sum_\gamma c_\gamma \text{Tr}(\Delta_\sigma^{1/2}(X^*)V_\gamma Y V_\gamma^*) \quad \text{GKS expansion} \\ &= \sum_\gamma c_\gamma \text{Tr}(V_\gamma^* \Delta_\sigma^{1/2}(X^*)V_\gamma Y) \quad \text{cyclicity of the trace} \\ &= \sum_\gamma c_\gamma \text{Tr}(V_\gamma \Delta_\sigma^{1/2}(X^*)V_\gamma^* Y) \quad \text{re-indexing} \\ &= \text{Tr}(L(\Delta_\sigma^{1/2}(X^*))Y) \\ &= \text{Tr}(\Delta_\sigma^{1/2}(LX^*)Y) \quad \text{commutation of } L \text{ with } \Delta_\sigma \\ &= \langle LX, Y \rangle_{1/2}. \end{aligned}$$

Hence, it turns out that L is self-adjoint with respect to the KMS inner product. According to a generalisation of theorem 4.28, which can be found in Carlen and Maas [6], it turns out that being self-adjoint with respect to an inner product with a particular value of s implies self-adjointness for all other s . Hence, also for the case $s = 1$ and thus we are done. \blacksquare

Similar to what we did for the general Lindblad form, we can work out the adjoint for ρ a

density operator to be given by

$$L^* \rho = \sum_{j \in J} \left(e^{-\omega_j/2} [V_j \rho, V_j^*] + e^{\omega_j/2} [V_j^*, \rho V_j] \right) \quad (4.72)$$

$$= \sum_{j \in J} e^{-\omega_j/2} \left([V_j \rho, V_j^*] + [V_j, V_j^* \rho] \right). \quad (4.73)$$

The result shown in theorem 4.30 shows that if a generator is self-adjoint with respect to the GNS inner product, STW and satisfies general generator conditions it has a simplified form. However, we do not know why a generator would be self-adjoint with respect to the GNS inner product. Therefore, it is interesting to figure out which physical systems actually poses this symmetry. Unfortunately, this question is outside the scope of this thesis, but can be considered for further research.

5

CONCLUSION

In this thesis Quantum Markov Semigroups and their generators were studied. These semigroups describe the evolution of operators or density matrices of open quantum systems. The generators of QMS have a general form described by the Lindblad equation, which was derived from both a physical and a mathematical perspective. Furthermore, the result of Carlen and Maas for a general form of a generator which commutes with the modular automorphisms group was generalised. This generalisation involved considering Hilbert spaces of countably infinite dimension instead of Hilbert spaces with dimension $n \in \mathbb{N}$. Furthermore, the modular automorphism group describes the time propagation of operators under a Hamiltonian induced by a density operator. It turned out that under the commutation the general form of the Lindblad equation simplified a great deal. However, we were only able to do so under multiple assumptions on the generators and their domain. We will reiterate the restrictions and mention what problems can be investigated by further research.

First of all, the general derivation of the Lindblad form for generators of QMS was done for the domain given by $B(\mathcal{H})$; the bounded operators, where \mathcal{H} can be countably infinite. However, in the generalisation of Carlen and Maas' result we only considered the domain $\mathcal{L}_3(\mathcal{H})$, which was defined to be the trace class operators with the identity and a compatible inner product. In this case the inner product defined on the trace class operators themselves was the regular Hilbert-Schmidt inner product and extended to the identity by defining it orthogonal to the trace class operators and normalising the inner product of the identity with itself to one. Unfortunately, this is a much more restrictive space than $B(\mathcal{H})$. Hence, for further research it is recommended to see if the results can be generalised for a more realistic inner product, i.e. not assuming the added identity is orthogonal to all other operators. An even better result would be to generalise the result from $\mathcal{L}_3(\mathcal{H})$ to $B(\mathcal{H})$. However, it should be noted that this probably cannot be done using the same proof tactics and techniques used in this thesis, since these strongly relied on the Hilbert-Schmidt inner product and the Hilbert space structure induced by it on the Hilbert-Schmidt/trace class operators.

Another point of consideration is the symmetry we assumed the generator obeyed. Namely, the self-adjointness with respect to the GNS inner product, which implied commutation with the modular automorphisms group. For this symmetry it is interesting to figure out what kind

of physical systems actually obey this particular requirement. That is which physical system actually have QMS generators that obey the simplified form.

Furthermore, we restricted the generators L to be both self-adjoint with respect to the inner product defined on $\mathcal{L}_3(\mathcal{H})$ and with respect to the GNS inner product. Additionally, we required L to be STW, or mapping strongly convergent sequences to weakly convergent sequences. These three requirements are complimentary to the conditions for L to be a generator of a QMS. However, only the self-adjointness with respect to the GNS inner product is required for L to have the proposed simplified Lindblad form in the finite dimensional case. Hence, for the infinite dimensional case we have two extra conditions. Both of these conditions are used to prove certain results. Nevertheless, as mentioned in the first paragraph, generalising the current result to $B(\mathcal{H})$ would probably require a different approach than the one taken in this thesis. Therefore, it is interesting to consider trying to lift the additional requirements on L to make the result even more general.

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REFERENCES

- [1] R. Alicki. “On the detailed balance condition for non-hamiltonian systems”. In: *Reports on Mathematical Physics* 10.2 (1976), pp. 249–258. ISSN: 00344877. DOI: 10.1016/0034-4877(76)90046-X.
- [2] R. Bhatia. *Positive Definite Matrices*. Princeton University Press, 2007. ISBN: 9788578110796. arXiv: arXiv:1011.1669v3.
- [3] C. A. Brasil, F. F. Fanchini, and R. de J. Napolitano. “A simple derivation of the Lindblad equation”. In: *Revista Brasileira de Ensino de Física* 35.1 (2013), pp. 1–11. ISSN: 01024744. DOI: 10.1590/s1806-11172013000100003. arXiv: 1110.2122.
- [4] O. Bratteli and D. W. Robinson. *Operator Algebras and Quantum Statistical Mechanics Vol 2*. 2nd ed. Springer US, 1997. ISBN: 3-540-61443-5.
- [5] H. -P. Breuer and F. Petruccione. *The theory of open quantum systems*. Oxford University Press, 2002. ISBN: 0 19 852063 8 1 3 5 7 9 10 8 6 4 2.
- [6] E. A. Carlen and J. Maas. “Gradient flow and entropy inequalities for quantum Markov semigroups with detailed balance”. In: *Journal of Functional Analysis* 273.5 (2017), pp. 1810–1869. ISSN: 10960783. DOI: 10.1016/j.jfa.2017.05.003. arXiv: 1609.01254. URL: <http://dx.doi.org/10.1016/j.jfa.2017.05.003>.
- [7] M. P. T. Caspers. *Lecture Notes on Quantum Information Theory*. 2021.
- [8] M. D. Choi. “Positive linear maps on operator algebras”. In: *Canada J. Math.* 24.3 (1972), pp. 520–529. ISSN: 00103616. DOI: 10.1007/BF01609408.
- [9] G. B. Folland. *A course in abstract harmonic analysis, second edition*. 1st ed. CRC Press, Inc., 1995. ISBN: 9781498727150.
- [10] S. Friedland. “Infinite dimensional generalizations of Choi’s Theorem”. In: *Special Matrices* 7.1 (2019), pp. 67–77. ISSN: 23007451. DOI: 10.1515/spma-2019-0006. arXiv: 1806.06938.
- [11] V. Gorini, A. Kossakowski, and E. C. G. Sudarshan. “Completely positive dynamical semigroups of N-level systems”. In: *Journal of Mathematical Physics* 17.5 (1975), pp. 821–825. ISSN: 00222488. DOI: 10.1063/1.522979.
- [12] S. J. Harris and S. K. Pandey. *Entanglement and non-locality*. 2016.
- [13] E. Hille and R. S. Phillips. *Functional Analysis and Semi-Groups*. 1957. DOI: 10.1201/9781439809266-4.
- [14] A. Kossakowski. “On quantum statistical mechanics of non-Hamiltonian systems”. In: *Reports on Mathematical Physics* 3.4 (1972), pp. 247–274. ISSN: 00344877. DOI: 10.1016/0034-4877(72)90010-9.
- [15] D. A. Lidar. *Lecture notes on the theory of open quantum systems*. 2019. arXiv: 1902.00967.

- [16] G. Lindblad. “On the generators of Quantum Dynamical Semigroups”. In: *Communications in Mathematical Physics* (1976). ISSN: 1540756X. DOI: 10.1080/10549811.2014.883998.
- [17] G. Lumer and R. S. Phillips. “Dissipative operators in a banach space”. In: *Pacific Journal of Mathematics* 11.2 (1961), pp. 679–698. ISSN: 00308730. DOI: 10.2140/pjm.1961.11.679.
- [18] D. Manzano. “A short introduction to the Lindblad master equation”. In: *AIP Advances* 10.2 (2020). ISSN: 21583226. DOI: 10.1063/1.5115323. arXiv: 1906.04478.
- [19] G. J. Murphy. *C*-Algebras and Operator Theory*. Academic Pres, Inc., 1990. ISBN: 0-12-511360-9.
- [20] S. Nayak. “A constructive proof of the derivation theorem”. In: *Mathematics Student* 88.3-4 (2019), pp. 119–124. ISSN: 00255742.
- [21] M. Nielsen and I. Chuang. *Quantum Computation and Quantum Information*. 10th ed. Cambridge University Press, 2010. ISBN: 9780511976667. DOI: 10.1017/CB09780511976667.
- [22] B. Russo and H. A. Dye. “A Note On Unitary Operators In C*-Algebras”. In: *Duke Mathematical Journal* 33.2 (1966), pp. 413–416. ISSN: 00127094. DOI: 10.1215/S0012-7094-66-03346-1.
- [23] S. Sakai. *C*-Algebras and W*-algebras*. Springer-Verlag Berlin Heidelberg, 1998. ISBN: 978-3-540-63633-5.
- [24] W. F. Stinespring. “Positive Functions on C*-Algebras”. In: *American Mathematical Society* 6.2 (1955), pp. 211–216.
- [25] D. M. Topping. *Lectures on Von Neumann Algebras*. Van Nostrand Reinhold Company, 1971. ISBN: 044208563X, 9780442085636.
- [26] J. Van Neerven. *An Introduction to Functional Analysis*. 2021.

A

ELEMENTARY TENSOR PRODUCT DEFINITIONS AND PROPOSITIONS

This section serves as an elementary introduction to tensor products, which only introduces the notions required in this paper. For further reading we recommend the reader to look at

Definition A.1. Let V and W be vector spaces. A tensor product of V and W is a pair $(V \otimes W, \otimes)$ of a vector space $V \otimes W$ and a bilinear map

$$\otimes : V \times W \rightarrow V \otimes W, \quad (v, w) \mapsto v \otimes w \quad (\text{A.1})$$

with the following universal property. For each bilinear map $\beta : V \times W \rightarrow U$ into a vector space U , there exists a unique linear map $\tilde{\beta} : V \otimes W \rightarrow U$ satisfying

$$\tilde{\beta}(v \otimes w) = \beta(v, w) \quad \text{for } v \in V, w \in W. \quad (\text{A.2})$$

It can be shown that this particular product is unique, furthermore to show its existence we use the following construction.

Proposition A.2. Let V and W be vector spaces and let $\mathcal{F}(V \times W)$ be the vector space with basis all Cartesian products $(v, w) \in V \times W$. Let $F \subseteq \mathcal{F}(V \times W)$ be the linear subspace spanned by the vectors.

$$(v, \lambda w) - \lambda(v, w), \quad (\lambda v, w) - \lambda(v, w) \quad (\text{A.3})$$

$$(v_1 + v_2, w) - (v_1, w) - (v_2, w), \quad (v, w_1 + w_2) - (v, w_1) - (v, w_2) \quad (\text{A.4})$$

Then we can define $V \otimes W$ as $\mathcal{F}(V \times W)/F$.

Considering the quotient we can deduce the following properties.

Property A.3. Let V and W be vector spaces then $\forall v \in V$ and $\forall w \in W$ we have the following:

$$(v_1 \otimes w) + (v_2 \otimes w) = ((v_1 + v_2) \otimes w) \quad (\text{A.5})$$

$$(v \otimes w_1) + (v \otimes w_2) = (v \otimes (w_1 + w_2)) \quad (\text{A.6})$$

$$(\lambda v \otimes w) = (v \otimes \lambda w) = \lambda(v \otimes w) \quad (\text{A.7})$$

We will now state another couple of important properties. If the reader is interested in the proofs for these particular properties, we refer them to

Property A.4. Let V and W be vector spaces and let $\mathcal{L}(V)$ and $\mathcal{L}(W)$ be the spaces of linear operators on V, W respectively. Furthermore, let $A \in \mathcal{L}(V)$ and $B \in \mathcal{L}(W)$ then we have the following:

- i) $\dim(V \otimes W) = \dim(V) \cdot \dim(W)$
- ii) $(A \otimes B)(v \otimes w) = Av \otimes Bw \quad \forall v \in V \text{ and } \forall w \in W.$
- iii) $\langle v \otimes w, x \otimes y \rangle = \langle v, x \rangle_V \langle w, y \rangle_W \quad \forall v, x \in V \text{ and } \forall w, y \in W.$
- iv) $\text{Tr}(A \otimes B) = \text{Tr}(A) \text{Tr}(B).$

The last important property of the tensor product that needs to be discussed is the Kronecker product. This is often used for products between linear operators that can be represented as matrices. It is defined as follows.

Definition A.5. Let A, B be linear operators with a matrix representation. Then the Kronecker product of $A \otimes B$ is defined as:

$$A \otimes B = \begin{pmatrix} a_{11}B & \dots & a_{1n}B \\ a_{21}B & \dots & a_{2n}B \\ \vdots & \ddots & \vdots \\ a_{n1}B & \dots & a_{nn}B \end{pmatrix} \quad (\text{A.8})$$

B

DIFFERENT WAYS OF LOOKING AT PRODUCTS OF MATRICES

Let $A, B, X \in M_2(\mathbb{C})$ then by employing the Kronecker product we can write

$$(A \otimes B^T) = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \otimes \begin{pmatrix} b_{11} & b_{21} \\ b_{12} & b_{22} \end{pmatrix} = \begin{pmatrix} a_{11}b_{11} & a_{11}b_{12} & a_{12}b_{11} & a_{12}b_{12} \\ a_{11}b_{21} & a_{11}b_{22} & a_{12}b_{21} & a_{12}b_{22} \\ a_{21}b_{11} & a_{21}b_{12} & a_{22}b_{11} & a_{22}b_{12} \\ a_{21}b_{21} & a_{21}b_{22} & a_{22}b_{21} & a_{22}b_{22} \end{pmatrix}. \quad (\text{B.1})$$

Then using this result we can write

$$\begin{aligned} (A \otimes B^T) \hat{X} &= \begin{pmatrix} a_{11}b_{11} & a_{11}b_{12} & a_{12}b_{11} & a_{12}b_{12} \\ a_{11}b_{21} & a_{11}b_{22} & a_{12}b_{21} & a_{12}b_{22} \\ a_{21}b_{11} & a_{21}b_{12} & a_{22}b_{11} & a_{22}b_{12} \\ a_{21}b_{21} & a_{21}b_{22} & a_{22}b_{21} & a_{22}b_{22} \end{pmatrix} \begin{pmatrix} x_{11} \\ x_{12} \\ x_{21} \\ x_{22} \end{pmatrix} \\ &= \begin{pmatrix} a_{11}b_{11}x_{11} + a_{11}b_{12}x_{12} + a_{12}b_{11}x_{21} + a_{12}b_{12}x_{22} \\ a_{11}b_{21}x_{11} + a_{11}b_{22}x_{12} + a_{12}b_{21}x_{21} + a_{12}b_{22}x_{22} \\ a_{21}b_{11}x_{11} + a_{21}b_{12}x_{12} + a_{22}b_{11}x_{21} + a_{22}b_{12}x_{22} \\ a_{21}b_{21}x_{11} + a_{21}b_{22}x_{12} + a_{22}b_{21}x_{21} + a_{22}b_{22}x_{22} \end{pmatrix}. \end{aligned}$$

This is the first result. Let us now move on to computing AXB

$$\begin{aligned} AXB &= \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \begin{pmatrix} x_{11} & x_{12} \\ x_{21} & x_{22} \end{pmatrix} \begin{pmatrix} b_{11} & b_{21} \\ b_{12} & b_{22} \end{pmatrix} \\ &= \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \begin{pmatrix} x_{11}b_{11} + x_{12}b_{12} & x_{11}b_{21} + x_{12}b_{22} \\ x_{21}b_{11} + x_{22}b_{12} & x_{21}b_{21} + x_{22}b_{22} \end{pmatrix} \\ &= \begin{pmatrix} a_{11}x_{11}b_{11} + a_{11}x_{12}b_{12} + a_{12}x_{21}b_{11} + a_{12}x_{22}b_{12} & a_{11}x_{11}b_{21} + a_{11}x_{12}b_{22} + a_{12}x_{21}b_{21} + a_{12}x_{22}b_{22} \\ a_{21}x_{11}b_{11} + a_{21}x_{12}b_{12} + a_{22}x_{21}b_{11} + a_{22}x_{22}b_{12} & a_{21}x_{11}b_{21} + a_{21}x_{12}b_{22} + a_{22}x_{21}b_{21} + a_{22}x_{22}b_{22} \end{pmatrix}. \end{aligned}$$

Reordering the terms in our last expression we see that these two operations yield the exact same result. Hence, both ways of computing are just a different way of looking at the same situation.