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Derivation of the Lindblad Equation for Open Quantum Systems and Its Application to Mathematical Modeling of the Process of Decision Making



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#### Abstract

In the theory of open quantum systems, a quantum Markovian master equation, the Lindblad equation, reveals the most general form for the generators of a quantum dynamical semigroup. In this thesis, we present the derivation of the Lindblad equation and several examples of Lindblad equations with their analytic and numerical solutions. The graphs of the numerical solutions illuminate the dynamics and the stabilization as time increases. The corresponding von Neumann entropies are also presented as graphs. Moreover, to illustrate the difference between the dynamics of open and isolated systems, we prove two theorems about the conditions for stabilization of the solutions of the von Neumann equation which describes the dynamics of the density matrix of open quantum systems. It shows that the von Neumann equation is not satisfied for modelling dynamics in the cognitive context in general. Instead, we use the Lindblad equation to model the mental dynamics of the players in the game of the 2-player prisoner's dilemma to explain the irrational behaviors of the players. The stabilizing solution will lead the mental dynamics to an equilibrium state, which is regarded as the termination of the comparison process for a decision maker. The resulting pure strategy is selected probabilistically by performing a quantum measurement. We also discuss two important concepts, quantum decoherence and quantum Darwinism. Finally, we mention a classical Neural Network Master Equation introduced by Cowan and plan our further works on an analogous version for the quantum neural network by using the Lindblad equation.

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#### 1 Introduction

Traditionally, the evolution within the framework of quantum mechanics (QM) focuses on the dynamics of microscopic particles. However, recently the mathematical formalism of QM started to be applied in cognitive science [44]-[70].

In classical game theory, the prisoner's dilemma is a canonical example [71]-[76], and the rational behavior for a player is to make the decision which approximates a Nash equilibrium. But in reality, there exists numerous experimental evidence of irrational behaviors. In the experiments in cognitive psychology which were performed by Tversky and Shafir [18], [19], the statistical data strongly indicate the existence of irrational behaviors. The irrational behavior for a player is to choose a strategy different from a Nash equilibrium. The classical game theory cannot explain it. One of the methods to explain the observed deviations from classical game theory (irrational behavior) is to apply the mathematical apparatus of QM<sup>1</sup>. In this thesis, we present numerical simulations of the Asano-Khrennikov-Ohya model [1], [2], [5], [4] which is a quantum-like decision making model. In this model, the mental dynamics for the player is described by Lindblad equation. As a result of the stabilization of its solution, the player makes a decision probabilistically. This combination of the Lindblad dynamics with asymptotic stabilization can be treated as a model of quantum measurement, as was proposed by W. Zurek [40]. In addition, we also present graphical forms of stabilizing solutions with the corresponding von Neumann entropies. We explain cognitive meanings related to behaviors of von Neumann entropies, and how decision making process is done with stabilizing solutions.

Before we get there, we present the derivation of the Lindblad equation. In quantum mechanics, the time evolution of a quantum state of an isolated system is described by the Schrödinger equation. The density operator describes a quantum system in a mixed state, and the Liouville-von Neumann equation describes the time evolution of the density operator for a closed quantum system. For an open quantum system, the dynamics involves the interaction with the environment. Due to the presence of infinitely many degrees of freedoms in the environment, its complete mathematical description will be very complicated, therefore we focus on the reduced density operator which can be obtained by taking the partial trace over the degrees of freedom for the environment. Alternatively, the reduced density operator at a certain time moment can be obtained with the aid of a dynamical map. With the variation of time, the set of all dynamical maps is a one parameter family, which forms a quantum dynamical semigroup [42], [43]. The Lindblad equation relates to the most general form of the generators of a quantum dynamical semigroup [16], [17].

We present some examples of the Lindblad equation with their numerical and/or analytic solutions. The corresponding von Neumann entropy for the density operator at different moments of time is presented as a graph. This mathematical modeling and numerical simulation for the Lindblad equation are important for the further mathematical modeling of cognitive behavior of the players in the process of decision making. Our examples illustrate in a simple graphical form (the output of the numerical simula-

<sup>&</sup>lt;sup>1</sup>We do not try to use quantum mechanics to model brain's functioning. We formally use the mathematical apparatus of QM to model information processing by cognitive systems.

tion) different types of behaviors for the solutions of the Lindblad equation. Moreover, to illustrate von Neumann equation is not appropriate for modelling of decision making process, we study condition of stabilization of the solutions of the von Neumann equation by proving two main theorems.

Then we introduce the basic concepts of classical game theory which are necessary to study existence of a Nash equilibrium [21], [22].

The main aim of this thesis is not only to present the details of deriving the Lindblad equation, but also to apply it to model the mental dynamics of a player in the game of Prisoner's Dilemma. The stabilized solution will lead the density operator to an equilibrium state, which is regarded as the action of termination of the comparison process for a decision maker. The resulting pure stategy is approached probabilistically by performing a quantum measurement. Moreover, we also discuss quantum decoherence and quantum Darwinism which are important for this quantum-like decision making model.

Finally, we mention Cowan's work on the classical Neural Network Master Equation and discuss the possibility to apply the Lindblad equation to quantum neural networks.

# **2** Open Quantum Systems and Quantum Master Equations

#### 2.1 Preliminaries

#### 2.1.1 Linear Algebra

A complex vector (linear) space *V* over the complex field *K* is a set of vectors satisfying the following properties

- 1. *V* is an Abelian additive group, i.e. there exists a fixed mapping  $V \times V \mapsto V$  denoted by  $(v, w) \mapsto v + w$ , and it satisfies the following axioms
  - (a) (u+v)+w=u+(v+w)
  - (b) u + v = v + u
  - (c) There exists a zero vector  $0 \in V$  such that u + 0 = u for all  $u \in V$
  - (d) For all  $u \in V$ , there exists a vector  $-u \in V$  such that u + (-u) = 0
- 2. There exists a fixed mapping  $K \times V \mapsto V$  denoted by  $(a, v) \mapsto av$ , it is satisfies the following axioms
  - (a) (ab)v = a(bv)
  - (b) a(v+w) = av + aw and (a+b)v = av + bv
  - (c) 1v = v

where  $a, b \in K$  and  $v, w \in V$ 

An inner product is a map  $(\cdot,\cdot): V \times V \mapsto \mathbb{C}$  satisfying the following properties

- 1.  $(x,y) = \overline{(y,z)}$
- 2. (x,y+z) = (x,y) + (x,z) and (x+y,z) = (x,z) + (y,z)
- 3. (cx,y) = c(x,y) and  $(x,cy) = \overline{(cy,x)} = \overline{c}(x,y)$
- 4.  $(x,x) \ge 0$  and (x,x) = 0 only when x is a zero vector.

A linear (vector) space equipped with an inner product is called an inner product space.

Remark. In this thesis, we consider only the complex linear (vector) spaces.

A norm p in a linear space V is a functional defined on V such that

- 1.  $p(x) \ge 0$
- 2. p(x) = 0 only if x = 0
- 3.  $p(\lambda x) = |\lambda| p(x)$  for all  $x \in V$  and  $\lambda \in \mathbb{C}$
- 4.  $p(x+y) \le p(x) + p(y)$  for all  $x, y \in V$

*Remark.* The norm of an element x in the linear space V is denoted by ||x||.

A linear space V equipped with a norm p(x) = ||x|| is called a normed linear space. The vectors  $(x_i)_{i \in I}$  are called linearly independent if there exists only trivial solution for the following equation

$$\sum_{i=1}^{n} c_i x_i = 0,\tag{1}$$

such that  $c_i = 0$  for all  $i \in I$ . The vectors are called linearly dependent if there exists non-trivial solution for the equation (1) such that at least one  $c_i \neq 0$ .

In an inner product space, the norm of a vector  $x \in V$  is defined by  $||x|| = \sqrt{(x,x)}$ . A basis of a vector space is an indexed family of vectors  $(x_i)_{i \in I}$  such that the vectors are linearly independent and span the vector space.

Two vectors  $x, y \in V$  are called orthogonal to each other if (x, y) = 0. An orthogonal basis of a vector space is the basis such that all the basis vectors are mutually orthogonal.

Given a squared matrix A, a non-zero vector v is called the eigenvector of A if it satisfies  $Av = \lambda v$ , where  $\lambda$  is called the eigenvalue of A corresponding to v. We can write the equation in the form

$$(A - \lambda I)v = 0 \tag{2}$$

where I is the identity matrix. To get the non-trivial solution for the homogeneous system, we have to use the equation  $\det(A - \lambda I) = 0$  to obtain a characteristic polynomial, where the roots are the eigenvalues. Then we can solve  $Av = \lambda v$  for all v corresponding to  $\lambda$ .

#### **Example 2.1.** Let us consider the Pauli matrices

$$\sigma_{x} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_{y} = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_{z} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$
 (3)

For  $\sigma_x$ , we have  $\det(\sigma_x - \lambda I) = \begin{vmatrix} -\lambda & 1 \\ 1 & -\lambda \end{vmatrix} = \lambda^2 - 1$ , where  $\lambda = \pm 1$ . By substituting the eigenvalues in the characteristic equation  $(\sigma_x - \lambda I)v = 0$  and solving it, we obtain the eigenvectors  $v_1 = \begin{pmatrix} 1 \\ -1 \end{pmatrix}, v_2 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$ .

For  $\sigma_y$ , we have  $\det(\sigma_y - \lambda I) = \begin{vmatrix} -\lambda & -i \\ i & -\lambda \end{vmatrix} = \lambda^2 - 1$ , where  $\lambda = \pm 1$ . By substituting the eigenvalues in the characteristic equation  $(\sigma_y - \lambda I)v = 0$  and solving it, we obtain the eigenvectors  $v_1 = \begin{pmatrix} 1 \\ -i \end{pmatrix}, v_2 = \begin{pmatrix} 1 \\ i \end{pmatrix}$ .

For  $\sigma_z$ , we have  $\det(\sigma_z - \lambda I) = \begin{vmatrix} 1 - \lambda & 0 \\ 0 & -1 - \lambda \end{vmatrix} = \lambda^2 - 1$ , where  $\lambda = \pm 1$ . By substituting the eigenvalues in the characteristic equation  $(\sigma_z - \lambda I)v = 0$  and solving it, we obtain the eigenvectors  $v_1 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, v_2 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ .

**Example 2.2.** For a spin-1/2 particle, we have the spin operator  $\sigma\theta = \cos(\theta)\sigma_x + \sin(\theta)\sigma_y$ . It has the matrix form

$$\sigma\theta = \begin{pmatrix} 0 & \cos(\theta) - i\sin(\theta) \\ \cos(\theta) + i\sin(\theta) & 0 \end{pmatrix} = \begin{pmatrix} 0 & e^{-i\theta} \\ e^{i\theta} & 0 \end{pmatrix}. \tag{4}$$

We have

$$\det(\sigma\theta - \lambda I) = \begin{vmatrix} -\lambda & e^{-i\theta} \\ e^{i\theta} & -\lambda \end{vmatrix} = \lambda^2 - 1$$
 (5)

Therefore, we have the eigenvalues  $\lambda=\pm 1$ . By substituting the eigenvalues in the characteristic equation  $(\sigma\theta-\lambda I)v=0$ , we obtain the corresponding eigenvectors  $v_1=\begin{pmatrix} -e^{-i\theta}\\1 \end{pmatrix}, v_2=\begin{pmatrix} e^{-i\theta}\\1 \end{pmatrix}$ . After normalization, the vectors are

$$v_1 = \begin{pmatrix} -\frac{e^{-i\theta}}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}, v_2 = \begin{pmatrix} \frac{e^{-i\theta}}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}. \tag{6}$$

A metric space is an ordered pair  $(X, \rho)$ , where X is a set and  $\rho$  is a function defined for all  $x, y \in X$ , i.e.  $\rho : X \times X \mapsto \mathbb{R}$ , if it satisfies

- 1.  $\rho(x,y) \ge 0$
- 2.  $\rho(x, y) = \rho(y, x)$
- 3.  $\rho(x,y) = 0$  if and only if x = y
- 4.  $\rho(x,z) \le \rho(x,y) + \rho(y,z)$

A metric space *X* is said to be complete if every Cauchy sequence  $\{x_n\}$  in *X* converges in *X*, i.e.  $\lim_{n\to\infty} ||x_{n+1}-x_n|| = 0$ .

*Remark.* A Cauchy sequence is a sequence such that for every positive number  $\varepsilon > 0$ , there exists an integer N such that  $||x_m - x_n|| < \varepsilon$ , where m, n > N.

We recall that any normed linear space is a metric space with the metric defined as  $\rho(x,y) = ||x-y||$ .

A Banach space  $\mathscr{B}$  is a complete normed linear space. A Hilbert space  $\mathscr{H}$  is a Banach space with the norm defined through the inner product, i.e.  $||x|| = \sqrt{(x,x)}$ .

Remark. Every Hilbert space is also a Banach space, but the converse is not necessary true.

**Example 2.3.** A complex vector space  $\mathbb{C}^n$  equippd with the inner product  $(x,y) = \sum_i x_i \overline{y_i}$ , where  $x, y \in \mathbb{C}^n$  is a finite dimensional Hilbert space.

A linear operator is a mapping  $A: \mathcal{H} \to \mathcal{H}$  such that  $A(\sum_i c_i x_i) = \sum_i c_i A(x_i)$  where  $x_i \in \mathcal{H}, c_i \in \mathbb{C}$ . An operator A is said to be non-negative if it satisfies  $(Ax, x) \geq 0$ , for all  $x \in \mathcal{H}$ .

A linear operator  $A: X \mapsto Y$  is said to be bounded between two normed linear spaces if it satisfies  $||Ax||_Y \le c||x||_X$  for some c > 0 and for all  $x \in X$ . The space of all bounded linear operators from X to Y is a normed linear space, denoted by B(X,Y).

*Remark.* The space of all bounded linear operators B(X,Y) is a Banach space if Y is a Banach space. See more details on bounded operators in the book [30].

The norm of a bounded linear operator A is defined by

$$||A|| = \sup_{\|x\| \le 1} ||Ax|| = \sup_{\|x\| = 1} ||Ax||$$
 (7)

*Remark.* A superoperator is a linear operator on the space of linear operators.

A semigroup of linear operators is a family  $(T(t))_{t\geq 0}$  of linear bounded operators on the Banach space X if it satisfies T(t+s)=T(t)T(s) for all  $t,s\geq 0$ , and T(0)=I.

The infinitesimal generator A of the semigroup T is defined by

$$Af = \lim_{t \to 0} A_t f = \lim_{t \to 0} \frac{1}{t} (T(t)f - f).$$
 (8)

An adjoint (Hermitian conjugate) of a linear operator A is a linear operator  $A^*$  such that  $(Ax,y)=(x,A^*y)$ , where  $x,y \in \mathcal{H}$ . A linear operator A is called self-adjoint (Hermitian) operator if it satisfies  $A=A^*$ . By fixing an orthogonal basis, we can represent a Hermitian operator by a Hermitian matrix such that it equals its conjugate transpose. We note that the adjoint  $A^*$  of the linear operator A is often denoted by  $A^{\dagger}$  in the context of physics.

*Remark.* Given a linear operator  $A: X \mapsto Y$  and suppose two corresponding bases  $(x_i)$  and  $(y_j)$ , respectively, then for every j, there exist complex numbers  $A_{ij}$  such that  $Ax_j = \sum_i A_{ij} y_i$ . The matrix  $(A_{ij})$  is called the matrix representation of the operator A.

Given an operator A on a Hilbert space  $\mathcal{H}$ , the trace of A is defined by

$$tr(A) = \sum_{i} A_{ii}.$$
 (9)

**Theorem 2.1.** The trace does not depend on the choice of an orthogonal basis.

*Proof.* Let A, B be the operators on a Hilbert space  $\mathcal{H}$ . By applying the definition of the trace, we have

$$\operatorname{tr}(AB) = \sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij} B_{ji} = \sum_{j=1}^{n} \sum_{i=1}^{n} B_{ji} A_{ij} = \operatorname{tr}(BA).$$
 (10)

For the different choices of the basis, it is done by the similarity transformation, i.e.  $B = P^{-1}AP$ , where P is a square invertible matrix. Since B is the matrix after the change of basis from A, thus we have

$$tr(B) = tr(P^{-1}AP) = tr(PP^{-1}A) = tr(A).$$
 (11)

Therefore, after change of basis, the trace does not change.

**Example 2.4.** Given a Pauli matrix 
$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$
, the trace is  $tr(\sigma_z) = 1 + (-1) = 0$ .

On the Hilbert space  $\mathscr{H}$ , a trace class operator is a bounded linear operator  $A: \mathscr{H} \mapsto \mathscr{H}$  if there exists a basis E such that  $\sum_{e \in E} (|A|e,e) < \infty$ . The space of all trace class operators on  $\mathscr{H}$  is denoted by  $B_1(\mathscr{H})$ .

A Hilbert-Schmidt operator on  $\mathcal{H}$  is an operator on  $\mathcal{H}$  such that  $|A|^2$  is trace class. Given two Hilbert-Schimidt operators F, G, their inner product is defined by

$$(F,G) \equiv \operatorname{tr}(F^{\dagger}G) = \sum_{i} (Fx_{i}, Gx_{i})$$
(12)

where  $\{x_i\}$  is an orthonormal basis of  $\mathcal{H}$ .

Two operators  $F_i$ ,  $F_j$  are orthogonal to each other if

$$(F_i, F_j) \equiv \operatorname{tr}(F_i^{\dagger} F_j) = \delta_{ij}, \tag{13}$$

where  $\delta_{ij}$  is the Kronecker delta function.

Remark. The Kronecker delta function is defined by

$$\delta_{ij} = \begin{cases} 0 & \text{if } i \neq j \\ 1 & \text{if } i = j \end{cases} \tag{14}$$

An operator U is called an unitary operator if it satisfies the equalities  $U^{\dagger}U=I$  and  $UU^{\dagger}=I$ .

**Example 2.5.** The Pauli matrix  $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$  is both Hermitian and unitary, since  $\sigma_x^{\dagger} \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}^2 = I$  and  $\sigma_x^{\dagger} = \sigma_x$ .

Given two Hilbert spaces  $\mathcal{H}_1, \mathcal{H}_2$ , their tensor product  $\mathcal{H}_1 \otimes \mathcal{H}_2$  is defined as a Hilbert space with the basis consisting of the formal expression  $\{x_i \otimes y_j\}$ , where  $\{x_i\}$  and  $\{y_j\}$  are the orthonormal bases for the Hilbert spaces  $\mathcal{H}_1, \mathcal{H}_2$ , respectively.

Generally, the tensor product satisfies the following properties

- 1.  $a(x \otimes y) = (ax) \otimes y = x \otimes (ay)$  for all  $a \in \mathbb{C}$  and  $x \in \mathcal{H}_1, y \in \mathcal{H}_2$
- 2.  $(x+y) \otimes z = x \otimes z + y \otimes z$  for all  $x, y \in \mathcal{H}_1$  and  $z \in \mathcal{H}_2$
- 3.  $x \otimes (z+w) = x \otimes z + x \otimes w$  for all  $x \in \mathcal{H}_1$  and  $z, w \in \mathcal{H}_2$

Given operators A and B acting on the vector spaces V and W and suppose x and y are vectors in V and W, the tensor product  $A \otimes B$  of two operators acting on the tensor product space  $V \otimes W$  is defined by

$$(A \otimes B)(x \otimes y) = (Ax) \otimes (By). \tag{15}$$

By fixing the orthonormal bases for two vector spaces, we can rewrite the equation (15) as

$$(A \otimes B)(\sum_{ij} \alpha_{ij} x_i \otimes y_j) = \sum_{ij} \alpha_{ij} A x_i \otimes B y_j$$
 (16)

where  $\{x_i\}$  and  $\{y_i\}$  are the orthonormal bases for the vector spaces V and W.

**Example 2.6.** Computationally, given two  $m \times n$  matrices A, B, their tensor product is

$$A \otimes B = \begin{pmatrix} a_{11}B & a_{12}B & \dots & a_{1n}B \\ a_{21}B & a_{22}B & \dots & a_{2n}B \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1}B & a_{m2}B & \dots & a_{mn}B \end{pmatrix}$$
(17)

In a tensor product space  $V \otimes W$ , we take two arbitrary vectors of the form  $p = \sum_{ij} \alpha_{ij} x_i \otimes y_j$  and  $q = \sum_{ij} \beta_{ij} x_i \otimes y_j$ , their inner product is defined by

$$(p,q) = (\sum_{ij} \alpha_{ij} x_i \otimes y_j, \sum_{ij} \beta_{ij} x_i \otimes y_j) = \sum_{ij} \overline{\alpha_{ij}} \beta_{ij} (x_i, x_i) (y_j, y_j)$$
(18)

We present a very short remark about  $W^*$ -algebra, since it will be used only once in the section of Lindblad equation.

*Remark.* A Banach algebra is an algebra B over the field C equipped with the norm such that B is a Banach space with the norm satisfying  $||xy|| \le ||x|| ||y||$ . An involution is a map  $x \mapsto x^*$  satisfying

- 1.  $(x^*)^* = x$
- 2.  $(x+y)^* = x^* + y^*$
- 3.  $(xy)^* = y^*x^*$
- 4.  $(\lambda x)^* = \overline{\lambda} x^*$ , where  $\lambda$  is a complex number.

A \*-algebra is the algebra with \*-involution. A  $C^*$ -algebra is a Banach \*-algebra with the property  $||x^*x|| = ||x||^2$ . The dual space  $B^*$  of a Banach space B is a space of linear maps  $f: B \mapsto \mathbb{C}$ .

*Example* 2.7. The algebra of all bounded operators  $B(\mathcal{H})$  on a Hilbert space  $\mathcal{H}$  is a  $C^*$ -algebra with the adjoint of the operators. To show it, we have to verify the equality  $||A^*A|| = ||A||^2$ , therefore we have to show  $||A^*A|| \le ||A||^2$  and  $||A||^2 \le ||A^*A||$  by using the Cauchy-Schwarz inequality, i.e.  $(x, y) \le ||x|| ||y||$ .

Firstly, we have

$$||A^*A|| = \sup_{\|x\| = \|y\| = 1} |(A^*Ax, y)|$$

$$= \sup_{\|x\| = \|y\| = 1} |(Ax, (A^*)^*y)| \le \sup_{\|x\| = \|y\| = 1} |||Ax|| ||Ay|| = ||A||^2$$
(20)

$$= \sup_{\|x\| = \|y\| = 1} |(Ax, (A^*)^*y)| \le \sup_{\|x\| = \|y\| = 1} |\|Ax\| \|Ay\| = \|A\|^2$$
 (20)

since  $(Ax, y) = (x, A^*y)$ .

Secondly, we have

$$||A||^{2} = \sup_{\|x\|=1} |(Ax, Ax)|$$

$$= \sup_{\|x\|=1} |(A^{*}Ax, x)| \le \sup_{\|x\|=1} ||A^{*}Ax|| = ||A^{*}A||$$
(21)

$$= \sup_{\|x\|=1} |(A^*Ax, x)| \le \sup_{\|x\|=1} |\|A^*Ax\| = \|A^*A\|$$
 (22)

Therefore, we conclude that  $||A^*A|| = ||A||^2$ .

Note that in an inner product space V with an orthonormal basis E, the Parseval's identity gives that

$$||v||^2 = (v, v) = \sum_{e \in E} |(v, e)|^2$$
 (23)

for all  $v \in V$ .

A W\*-algebra is a C\*-algebra  $\mathscr A$  such that  $\mathscr A$  is a dual space as a Banach space. It means there exist a Banach space  $A_*$  and its coupled dual Banach space  $(A_*)^*$  such that  $(A_*)^* = A$ . And the Banach space  $\mathscr{A}_*$  is called a pre-dual of  $\mathscr{A}$ .

Example 2.8. Let  $B(\mathcal{H})$  be an algebra of all bounded operators on a Hilbert space  $\mathcal{H}$ . As it is shown in the Example 2.7, the algebra  $B(\mathcal{H})$  is a  $C^*$ -algebra and it has a predual which is the space  $B_1(\mathcal{H})$  of the trace class operators. By definition, the algebra  $B(\mathcal{H})$  is a  $W^*$ -algebra.

We introduce the ultraweak convergence which will be used in the section on Lindblad equation.

A directed set I is a set with the preordering property and for every pair of elements, there exists an upper bound, i.e. for any two elements  $i_0, i_1 \in I$ , there exists an element  $i \in I$  such that  $i_0 \le i$  and  $i_1 \le i$ . Let X be a topological space and I be a directed set, a net  $(x_i)_{i \in I}$  in X is a mapping  $N : I \mapsto X$ .

A net  $(x_i)_{i \in I}$  is convergent to x if for every neighborhood U, there exists an index  $i(U) \in I$  such that for all  $i \ge i(U)$  where  $i \in I$ , we have  $x_i \in U$ .

Let  $B(\mathcal{H})$  be a space of the bounded operators on the Hilbert space  $\mathcal{H}$ , a net  $(f_i)_{i\in I}$  in  $B(\mathcal{H})$  is strongly convergent to  $f\in B(\mathcal{H})$  if for all  $v\in \mathcal{H}$ , the net  $(f_i)_{i\in I}$  is convergent to f(v) in  $\mathcal{H}$ . A net  $(f_i)_{i\in I}$  in  $B(\mathcal{H})$  is weakly convergent to  $f\in B(\mathcal{H})$  if for all pairs of  $v, w \in \mathcal{H}$ , the net  $(\langle f_i(v), w \rangle)_{i \in I}$  is convergent to  $(\langle f(v), w \rangle)$  in  $\mathbb{C}$ .

A net  $(f_i)_{i\in I}$  in  $B(\mathscr{H})$  is ultraweakly convergent to  $f\in B(\mathscr{H})$  if for all pairs of sequences  $(x_n)_{n\geq 0}, (y_n)_{n\geq 0}$  of elements in  $\mathscr{H}$  where  $\sum_{n\geq 0}\|x\|^2 < \infty$  and  $\sum_{n\geq 0}\|y\|^2 < \infty$ , the net  $\sum_{n>0}|\langle f_i(x_n), y_n\rangle|$  is convergent to  $\sum_{n>0}|\langle f(x_n), y_n\rangle|$ .

In order to smoothly introduce the von Neumann entropy in the next section, we define the operator exponential and operator logarithm. By fixing a basis, they can be represented by the matrix exponential and matrix logarithm, respectively. They play an important role in the theories of Lie groups and Lie algebras.

**Definition 2.1.** The exponential of a bounded linear operator *A* in a Banach space is defined by using power series as follows

$$e^A = E + A + \frac{A^2}{2!} + \dots = \sum_{i=0}^{\infty} \frac{1}{i!} A^i,$$
 (24)

where E is the identity operator, i.e. Ex = x.

By fixing a basis of the operator, the operator exponential has matrix representation.

**Definition 2.2.** The exponential of an  $n \times n$  real or complex matrix X is defined by using power series as follows

$$e^{X} = \sum_{i=0}^{\infty} \frac{1}{i!} X^{i}, \tag{25}$$

where  $e^0 = I$ .

Let us consider some examples about how to compute the exponential of a squared matrix.

Let X be an  $n \times n$  real or complex matrix and it is diagonalizable over  $\mathbb{C}$ , i.e. there exists an invertible complex matrix C such that  $X = CDC^{-1}$ , where  $D = \begin{pmatrix} \lambda_1 & 0 \\ & \ddots & \\ 0 & & \lambda_n \end{pmatrix}$ .

As it was shown in Hall's book [41], the exponential of X is in the form

$$e^{X} = C \begin{pmatrix} e^{\lambda_{1}} & 0 \\ & \ddots & \\ 0 & e^{\lambda_{n}} \end{pmatrix} C^{-1}$$
 (26)

Therefore, we can explicitly compute the exponential of X.

**Example 2.9.** Given a matrix  $X = \begin{pmatrix} 0 & -a \\ a & 0 \end{pmatrix}$ , the eigenvectors of X are  $\begin{pmatrix} 1 \\ i \end{pmatrix}$ ,  $\begin{pmatrix} i \\ 1 \end{pmatrix}$  and the corresponding eigenvalues are -ia, ia. We have an invertible matrix  $C = \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix}$  and  $D = C^{-1}XC$  is a diagonal matrix. Therefore, we have  $X = CDC^{-1}$  and

$$e^{X} = \begin{pmatrix} 1 & i \\ i & 1 \end{pmatrix} \begin{pmatrix} e^{-ia} & 0 \\ 0 & e^{ia} \end{pmatrix} \begin{pmatrix} \frac{1}{2} & -\frac{i}{2} \\ -\frac{i}{2} & \frac{1}{2} \end{pmatrix}$$
$$= \begin{pmatrix} \cos(a) & -\sin(a) \\ \sin(a) & \cos(a) \end{pmatrix}$$

*Remark.* The matrix  $\begin{pmatrix} \cos(a) & -\sin(a) \\ \sin(a) & \cos(a) \end{pmatrix}$  is called rotation matrix.

Let *X* be an  $n \times n$  matrix, it is said to be nilpotent if  $X^i = 0$  for some positive integer *i*. Obviously, for all j > i, we have  $X^j = 0$ . It allows us to explicitly compute the the exponential.

**Example 2.10.** Given a matrix  $X = \begin{pmatrix} 0 & a & b \\ 0 & 0 & c \\ 0 & 0 & 0 \end{pmatrix}$ . We have  $X^2 = \begin{pmatrix} 0 & 0 & ac \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$ , and  $X^3 = 0$ . Therefore,

$$\begin{split} e^X &= \sum_{i=0}^{\infty} \frac{1}{i!} X^i \\ &= \sum_{i=0}^{2} \frac{1}{i!} X^i \\ &= \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} + \begin{pmatrix} 0 & a & b \\ 0 & 0 & c \\ 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & \frac{ac}{2} \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \\ &= \begin{pmatrix} 1 & a & b + \frac{ac}{2} \\ 0 & 1 & c \\ 0 & 0 & 1 \end{pmatrix} \end{split}$$

**Theorem 2.2.** Let X be an  $n \times n$  complex matrix. There exists two unique matrices S, N such that X = S + N and SN = NS, where S is diagonalizable and N is nilpotent, .

*Remark.* The expression X = S + N is called SN decomposition. See the proof of this theorem in Hall's book [41].

Let X be an general  $n \times n$  matrix. It has an SN decomposition as it is shown in Theorem 2.2. Therefore, we can write the exponential of X in the form

$$e^X = e^{S+N} = e^S e^N,$$
 (27)

where  $e^S$  and  $e^N$  can be computed explicitly as is shown in previous two examples.

**Example 2.11.** Given a matrix  $X = \begin{pmatrix} a & b \\ 0 & a \end{pmatrix}$ , we have

$$X = \begin{pmatrix} a & 0 \\ 0 & a \end{pmatrix} + \begin{pmatrix} 0 & b \\ 0 & 0 \end{pmatrix} \tag{28}$$

Therefore,

$$e^{X} = \begin{pmatrix} e^{a} & 0 \\ 0 & e^{a} \end{pmatrix} \begin{pmatrix} 1 & b \\ 0 & 1 \end{pmatrix}$$
$$= \begin{pmatrix} e^{a} & e^{a}b \\ 0 & e^{a} \end{pmatrix}$$

An inverse function of the exponential of a matrix is the matrix logarithm.

#### **Lemma 2.3.** The function

$$\log z = \sum_{m=1}^{\infty} (-1)^{m+1} \frac{(z-1)^m}{m}$$
 (29)

is defined and analytic in a circle of radius 1 about z = 1.

For all z with |z-1| < 1, we have  $e^{\log z} = z$ .

For all u with  $|u| < \log 2$ , we have  $|e^u - 1| < 1$  and  $\log e^u = u$ .

The series has the radius of convergence 1 with the complex analytic function on the disk  $\{|z-1| < 1\}$ .

Analogously, we can define the logarithm of an operator.

**Definition 2.3.** The logarithm of a bounded linear operator A in a Banach space is defined by

$$\log A = \sum_{m=1}^{\infty} (-1)^{m+1} \frac{(A-E)^m}{m}$$
 (30)

whenever the series converges in the space of the bounded linear operators, and E is the identity operator, i.e. Ex = x.

Due to the radius of convergence 1 for the complex valued series, then the operator valued series is convergent if ||A - E|| < 1.

By fixing a basis of the operator, the operator logarithm has the matrix representation.

#### **Definition 2.4.** The logarithm of an $n \times n$ matrix X is defined by

$$\log X = \sum_{m=1}^{\infty} (-1)^{m+1} \frac{(X-I)^m}{m}$$
 (31)

whenever the series converges.

Due to the radius of convergence 1 for the complex valued series, then the matrix valued series is convergent if ||X - I|| < 1.

For further details of the matrix logarithms and the related theories of Lie algebras, we refer to the book of Hall[41].

See more details on linear algebra in the books of Lax [30], Hoffman [31], Dym [32], Roman [33] and Greub [34]

#### 2.1.2 Quantum Mechanics

The serious development of quantum mechanics started from Heisenberg's matrix mechanics [12], [13], [14] and Schrödinger's wave mechanics [15] in 1925-1926. After that, Born proposed that the wave function can be interpreted statistically by using probability theory to interprete the observations. This approach developed into the Copenhagen interpretation of quantum mechanics.

*Remark.* We are proceeding in the finite dimensional case so that we can deal with matrices instead of operators.

*Remark.* In quantum mechanics, a column vector is denoted by  $|x\rangle$ , a row vector is denoted by  $\langle y|$ . The inner product of two arbitrary vectors  $|v\rangle$ ,  $|w\rangle \in \mathscr{H}$  is denoted by  $\langle v|w\rangle$ . The quantum observables are given by Hermitian matrices. The matrix elements  $(e_i,Ae_j)$  can be written in an alternative form  $\langle e_i|A|e_j\rangle$ . It is called Bra-ket (or Dirac) notation.

A pure quantum state can be represented as a normalized vector, i.e.  $\langle \phi | \phi \rangle = 1$ , where  $|\phi\rangle \in \mathcal{H}$ . The operator  $P_{\phi} = |\phi\rangle \langle \phi|$  projects a vector onto the pure state  $|\phi\rangle$ , where  $|\phi\rangle \langle \phi|$  is the Dirac notation for the projection operator. Any projector is a Hermitian, non-negative, trace-one operator and its square equals to itself.

For the coordinates of a quantum state vector, its squared absolute values are represented as probabilities according to the Born's rule.

Given a quantum observable which is described by a Hermitian matrix A, it has the eigenvalues  $\lambda_j$  and eigenvectors  $e_j$  in the form  $Ae_j = \lambda_j e_j$ .

Additionally, every pure state  $\psi$  can be written in terms of orthonormal basis vectors (eigenvectors) of A as follows  $\psi = \sum_j c_j e_j$ , where  $\sum_j |c_j|^2 = 1$ . In a measurement of the quantum observable, the values  $\lambda_j$  can only be observed probabilistically according to the quantum postulation i.e.

$$P(A_{\psi} = \lambda_i) = |c_i|^2 = |\langle e_i | \psi \rangle|^2. \tag{32}$$

Note that it is not possible to predict which exact value of  $\lambda_j$  will be obtained.

We consider the state of a quantum system as a vector of expectation values for every bounded linear operator such that the mean value of the observable *A* is defined by

$$\langle A \rangle_{\psi} = \sum_{j} \lambda_{j} p_{j}, \tag{33}$$

where  $p_i = P_{\Psi}(A = \lambda_i)$ .

The density operator  $\rho$  is a self-adjoint, non-negative and trace-one operator.

Given a composite quantum system with the state space  $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$  and let A be an operator on  $\mathcal{H}$ , the partial trace of A over  $\mathcal{H}_2$  is defined by

$$\operatorname{tr}_{2}A = \sum_{i} (I \otimes \langle \psi_{i} |) A(I \otimes | \psi_{i} \rangle), \tag{34}$$

where  $\{|\psi_i\rangle\}$  is an orthonormal basis in  $\mathcal{H}_1$ . The partial trace can be considered as a generalization of the trace, it is an operator-valued function.

**Example 2.12.** Consider a Bell state  $|\psi\rangle_{AB} = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$ . We have the corresponding density operator in the form

$$\rho_{AB} = \frac{1}{2} (|00\rangle \langle 00| + |00\rangle \langle 11| + |11\rangle \langle 00| + |11\rangle \langle 11|). \tag{35}$$

We can calculate the partial trace as follows

$$\begin{split} \operatorname{tr}_2 &= \frac{1}{2} (\operatorname{tr}(|00\rangle \langle 00|) + \operatorname{tr}(|00\rangle \langle 11|) + \operatorname{tr}(|11\rangle \langle 00|) + \operatorname{tr}(|11\rangle \langle 11|)) \\ &= \frac{1}{2} (|0\rangle \langle 0| \langle 0|0\rangle + |0\rangle \langle 1| \langle 1|0\rangle + |1\rangle \langle 0| \langle 0|0\rangle + |1\rangle \langle 1| \langle 1|1\rangle) \\ &= \frac{1}{2} (|0\rangle \langle 0| + |1\rangle \langle 1|) \\ &= \frac{I}{2} \end{split}$$

The von Neumann entropy measures the uncertainty presented in the density operator. Let  $\rho$  be the density operator, the von Neumann entropy of  $\rho$  is defined by

$$S(\rho) = -\operatorname{tr}(\rho \log \rho). \tag{36}$$

Alternatively, it can be reformulated as

$$S(\rho) = -\sum_{x} \lambda_{x} \log \lambda_{x}, \tag{37}$$

where  $\lambda_x$  are the eigenvalues of  $\rho$  and  $0 \log 0 = 0$ .

**Example 2.13.** Given a density matrix  $\rho = \begin{pmatrix} \frac{2}{5} & \frac{\sqrt{6}}{5} \\ \frac{\sqrt{6}}{5} & \frac{3}{5} \end{pmatrix}$ , where the eigenvalues are 0,1. We can compute its von Neumann entropy

$$S(\rho) = -(0\log(0) + 1\log(1)) = 0 \tag{38}$$

See more details on quantum mechanics in the books of Dirac [8], Sakurai [9] and von Neumann [29].

#### 2.2 Closed and Open Quantum Systems

The unitary time evolution of the quantum state  $|\psi(t)\rangle$  of a closed system is described by the Schrödinger equation,

$$i\hbar \frac{d}{dt} |\psi(t)\rangle = H(t) |\psi(t)\rangle$$
 (39)

where  $\hbar$  is the Plank's constant and H is the Hamiltonian which is the Hermitian operator describing the total energy of the quantum system.

The solution can be written in terms of unitary time evolution in the form  $|\psi(t)\rangle = U(t,t_0)|\psi(t_0)\rangle$ , where  $U(t,t_0):|\psi(t_0)\rangle \to |\psi(t)\rangle$  is the operator mapping the quantum state at an initial time  $t_0$  to the quantum state at time t, and it follows

$$\langle \psi(t_0) | U^{\dagger}(t, t_0) U(t, t_0) | \psi(t_0) \rangle = \langle \psi(t_0) | I | \psi(t_0) \rangle \tag{40}$$

$$= \langle \psi(t_0) \, | \, \psi(t_0) \rangle \tag{41}$$

$$=1, (42)$$

since the operator  $U(t,t_0)$  is unitary and the state vector is normalized.

**Example 2.14.** Let  $H = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$  be a time independent Hamiltonian and let us assume the Plank's constant to be 1, i.e.  $\hbar = 1$ . And consider a quantum state  $|\psi(t)\rangle = \begin{pmatrix} \psi_0(t) \\ \psi_1(t) \end{pmatrix}$ . We can rewrite the Schrödinger equation in the form of the corresponding system of linear ordinary differential equations as follows

$$\begin{cases} \frac{d}{dt}\psi_0(t) = -i\psi_1(t) \\ \frac{d}{dt}\psi_1(t) = -i\psi_0(t) \end{cases}$$
(43)

The analytic solutions are

$$\begin{cases} \psi_0(t) = \psi_0(0)\cos(t) - i\psi_1(0)\sin(t) \\ \psi_1(t) = \psi_1(0)\cos(t) - i\psi_0(0)\sin(t) \end{cases}$$
(44)

where  $\psi_0(0), \psi_1(0)$  are the initial conditions.

Analogously, we can consider an operator equation by substituting the form of the quantum state in terms of the unitary time evolution operator into the equation (39) as follows

$$i\hbar \frac{\partial}{\partial t} U(t, t_0) = H(t)U(t, t_0).$$
 (45)

For the time independent Hamiltonian H, we have

$$U(t,t_0) = \exp[-\frac{i}{\hbar}H(t-t_0)]. \tag{46}$$

For the time dependent Hamiltonian H, we have

$$U(t,t_0) = \mathbf{T}_{\leftarrow} \exp\left[-\frac{i}{\hbar} \int_{t_0}^t ds H(s)\right]. \tag{47}$$

where  $T_{\leftarrow}$  is the time ordering operator defined by:

$$T(A(t_a)B(t_b)) = \begin{cases} A(t_a)B(t_b), & \text{if } t_a > t_b \\ B(t_b)A(t_a), & \text{if } t_b > t_a \end{cases}$$
(48)

where  $A(t_a)$ ,  $B(t_b)$  are the operators and  $t_a$ ,  $t_b$  are the time variables for two operators, respectively.

*Remark.* Note that the form of an unitary time evolution operator in terms of the Hamiltonian H is in the form of operator exponential. By fixing an orthonormal basis, the operator exponential can be represented as the matrix exponential.

**Example 2.15.** Let  $H = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$  be a time independent Hamiltonian and let us assume the Plank's constant to be 1, i.e.  $\hbar = 1$ . The corresponding time evolution operator is  $U = \begin{pmatrix} \cos(t) & -i\sin(t) \\ -i\sin(t) & \cos(t) \end{pmatrix}$  such that

$$U^{\dagger}U = \begin{pmatrix} \cos(t) & i\sin(t) \\ i\sin(t) & \cos(t) \end{pmatrix} \begin{pmatrix} \cos(t) & -i\sin(t) \\ -i\sin(t) & \cos(t) \end{pmatrix} = I \tag{49}$$

The density operator for a quantum system in a mixed state at an intial time  $t_0$  is  $\rho(t_0) = \sum_{\alpha} w_{\alpha} |\psi_{\alpha}(t_0)\rangle \langle \psi_{\alpha}(t_0)|$ . Each of the pure states evolves in time driven by the Schrödinger equation, therefore it gives the density operator at time t in the form

$$\rho(t) = \sum_{\alpha} w_{\alpha} U(t, t_0) |\psi_{\alpha}(t_0)\rangle \langle \psi_{\alpha}(t_0)| U \dagger (t, t_0)$$
(50)

$$=U(t,t_0)\rho(t_0)U\dagger(t,t_0). \tag{51}$$

**Example 2.16.** Let us consider two quantum states  $|\psi_1(t_0)\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$  and  $|\psi_2(t_0)\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ 

 $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$  and  $w_1 = \frac{1}{3}, w_2 = \frac{2}{3}$ . The density matrix at intial time is

$$\rho(t_0) = \sum_{\alpha} w_{\alpha} |\psi_{\alpha}(t_0)\rangle \langle \psi_{\alpha}(t_0)|$$
 (52)

$$= \begin{pmatrix} \frac{1}{3} & 0\\ 0 & \frac{2}{3} \end{pmatrix}. \tag{53}$$

Consider a time independent Hamiltonian  $H = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$  with the corresponding unitary time evolution operator in the matrix form  $U = \begin{pmatrix} \cos(t) & -i\sin(t) \\ -i\sin(t) & \cos(t) \end{pmatrix}$ .

We have the density matrix at time t in the form

$$\rho(t) = U\rho(t_0)U\dagger \tag{54}$$

$$= \begin{pmatrix} \cos(t) & -i\sin(t) \\ -i\sin(t) & \cos(t) \end{pmatrix} \begin{pmatrix} \frac{1}{3} & 0 \\ 0 & \frac{2}{3} \end{pmatrix} \begin{pmatrix} \cos(t) & i\sin(t) \\ i\sin(t) & \cos(t) \end{pmatrix}$$
(55)

$$= \begin{pmatrix} \cos(t) & -i\sin(t) \\ -i\sin(t) & \cos(t) \end{pmatrix} \begin{pmatrix} \frac{1}{3} & 0 \\ 0 & \frac{2}{3} \end{pmatrix} \begin{pmatrix} \cos(t) & i\sin(t) \\ i\sin(t) & \cos(t) \end{pmatrix}$$

$$= \begin{pmatrix} \frac{1+\sin^{2}(t)}{3} & -i\frac{\sin(t)\cos(t)}{3} \\ i\frac{\sin(t)\cos(t)}{3} & \frac{1+\cos^{2}(t)}{3} \end{pmatrix}.$$

$$(56)$$

Then we consider the dynamics of the density operator with the Hamiltonian H as follows

$$\frac{d}{dt}\rho(t) = \frac{d}{dt}U(t,t_0)\rho(t_0)U\dagger(t,t_0) + U(t,t_0)\rho(t_0)\frac{d}{dt}U\dagger(t,t_0)$$
(57)

$$= -\frac{i}{\hbar}H(t)U(t,t_0)\rho(t_0)U\dagger(t,t_0) + U(t,t_0)\rho(t_0)\frac{i}{\hbar}U\dagger(t,t_0)H(t)$$
 (58)

$$= -\frac{i}{\hbar}H(t)\rho(t) + \frac{i}{\hbar}\rho(t)H(t)$$
(59)

$$=: -\frac{i}{\hbar}[H(t), \rho(t)]. \tag{60}$$

The equation (60) we obtained is the famous Liouville-von Neumann equation for the closed quantum system. We can rewrite it in a more compact form  $\frac{d}{dt}\rho(t) = \mathcal{L}(t)\rho(t)$ , where  $\mathcal{L}(t)$  is the Liouville superoperator. It has the analogue solutions such that

$$\rho(t) = \exp[\mathcal{L}(t - t_0)]\rho(t_0) \tag{61}$$

is for the time independent Hamiltonian and

$$\rho(t) = \mathbf{T}_{\leftarrow} \exp\left[\int_{t_0}^t ds \mathcal{L}(s)\right] \rho(t_0) \tag{62}$$

is for the time dependent Hamiltonian where  $T_{\leftarrow}$  is the time ordering operator defined in (48).

**Example 2.17.** Given a time independent Hamiltonian  $H = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$  and the density

matrix  $\rho(t) = \begin{pmatrix} \frac{1}{3} & 0 \\ 0 & \frac{2}{3} \end{pmatrix}$  at time t and we assume the Plank's constant to be 1, i.e.  $\hbar = 1$ . We have the von Neumann equation in the form

$$\frac{d}{dt}\rho(t) = -i[H,\rho(t)] \tag{63}$$

$$= -i(H\rho(t) - \rho(t)H) \tag{64}$$

$$=-i\begin{pmatrix}0&1\\1&0\end{pmatrix}\begin{pmatrix}\frac{1}{3}&0\\0&\frac{2}{2}\end{pmatrix}+i\begin{pmatrix}\frac{1}{3}&0\\0&\frac{2}{2}\end{pmatrix}\begin{pmatrix}0&1\\1&0\end{pmatrix}$$
 (65)

$$= \begin{pmatrix} 0 & -\frac{i}{3} \\ \frac{i}{3} & 0 \end{pmatrix}. \tag{66}$$

In quantum mechanics, the Schrödinger picture indicates that the quantum states evolve in time, but the observables (operators) are constant. Conversely, the Heisenburg pictures indicates that the observables (operators) evolve in time, but the quantum states are constant. And the interaction picture indicates that both of the observables (operators) and the quantum states envolve in time.

The Liouville-von Neumann equation describes the dynamics of the density operator in the Schrödinger picture.

A transformation from the Schrödinger picture operator A(t) to the Heisenberg picture operator  $A_H(t)$  in terms of the unitary time evolution operator is in the form

$$A_H(t) = U^{\dagger}(t, t_0) A(t) U(t, t_0) \tag{67}$$

where  $A(t_0) = A_H(t_0)$  and we allow the Schrödinger picture operator A(t) depending on time explicitly.

Let us derive the dynamics of an arbitrary operator in the Heisenberg picture as follows

$$\begin{split} \frac{d}{dt}A_{H}(t) &= \frac{\partial}{\partial t}U^{\dagger}(t,t_{0})A(t)U(t,t_{0}) + U^{\dagger}(t,t_{0})\frac{\partial}{\partial t}A(t)U(t,t_{0}) + U^{\dagger}(t,t_{0})A(t)\frac{\partial}{\partial t}U(t,t_{0}) \\ &= \frac{i}{\hbar}U^{\dagger}(t,t_{0})H(t)A(t)U(t,t_{0}) - \frac{i}{\hbar}U^{\dagger}(t,t_{0})A(t)H(t)U(t,t_{0}) + U^{\dagger}(t,t_{0})\frac{\partial}{\partial t}A(t)U(t,t_{0}) \\ &= \frac{i}{\hbar}H_{H}(t)A_{H}(t) - \frac{i}{\hbar}A_{H}(t)H_{H}(t) + \frac{\partial}{\partial t}A_{H}(t) \\ &= \frac{i}{\hbar}[H_{H}(t),A_{H}(t)] + \frac{\partial}{\partial t}A_{H}(t) \end{split}$$

Specifically, let A = H, we have  $\frac{d}{dt}H_H(t) = \frac{i}{\hbar}[H_H(t), H_H(t)] + \frac{\partial}{\partial t}H_H(t) = \frac{\partial}{\partial t}H_H(t)$ . For an isolated system  $\frac{\partial}{\partial t}H_H(t) = 0$ , we have  $\frac{d}{dt}H_H(t) = 0$ . It indicates that the Hamiltonian in the Heisenberg pictures is constant.

For the interaction picture, we separate the Hamiltonian into two parts  $H(t) = H_0 + H_I(t)$  where  $H_0$  is the sum of the energies when ignoring the interaction between two systems with the time independence, and  $H_I(t)$  is the interaction Hamiltonian. The expection value of the Schrödinger observable is  $\langle A(t) \rangle = \text{tr}\{A(t)U(t,t_0)\rho(t_0)U^{\dagger}(t,t_0)\}$ .

Let us introduce two time evolution operators

$$U_0(t,t_0) = \exp[-iH_0(t-t_0)] \tag{68}$$

and

$$U_I(t,t_0) = U_0^{\dagger}(t,t_0)U(t,t_0). \tag{69}$$

It gives

$$\langle A(t) \rangle = \text{tr}\{U_0^{\dagger}(t, t_0)A(t)U_0(t, t_0)U_I(t, t_0)\rho(t_0)U_I^{\dagger}(t, t_0)\}$$
 (70)

$$= \operatorname{tr}\{A_I(t)\rho_I(t)\}. \tag{71}$$

The time evolution in the interaction picture is driven by the free Hamiltonian part  $H_0$ . When  $\hat{H}_I(t) = 0$ , we have  $U_0(t,t_0) = U(t,t_0)$  and  $U_I(t,t_0) = I$ , then it is in the Heisenberg picture. Conversely, when  $H_0(t) = 0$ , we have  $U_0(t,t_0) = I$  and  $U_I(t,t_0) = U(t,t_0)$ , then it is in the Schrödinger picture. We can see the Schrödinger picture and Heisenburg picture are opposite to each other. The dynamics of the interaction picture time evolution operator is

$$i\frac{\partial}{\partial t}U_I(t,t_0) = H_I(t)U_I(t,t_0)$$
(72)

where  $H_I(t) = U_0^{\dagger}(t,t_0)\hat{H}_I(t)U_0(t,t_0)$ . Then we have the interaction picture Liouvillevon Neumann equation as follows

$$\frac{d}{dt}\rho_I(t) = -i[H_I(t), \rho_I(t)]. \tag{73}$$

It has an equivalent integral form as follows

$$\rho_I(t) = \rho_I(t_0) - i \int_{t_0}^t ds [H_I(s), \rho_I(s)]. \tag{74}$$

For an open quantum system, the total system is regarded as a combination of the subsystems S+B, where S is a quantum system and B is the coupled environment which is also a quantum system. The dynamics of the subsystem S is driven by the self-dynamics and the environment interaction. The reduced system dynamics is the subsystem dynamics for S induced by the total system Hamiltonian evolution. Given the system Hilbert space  $\mathscr{H}_S$  and the environment Hilbert space  $\mathscr{H}_B$ , the total system Hilbert space is defined by  $\mathscr{H}_S \otimes \mathscr{H}_B$ . The total Hamiltonians has the form  $H(t) = H_S \otimes I_B + I_S \otimes H_B + \hat{H}_I(t)$ , where  $H_S$  is the system Hamiltonian ,  $H_B$  is the environment

Hamiltonian and  $\hat{H}_I(t)$  is the interaction Hamiltonian. A reservoir is the environment with infinite number of degrees of freedom, and the continuum is formed from the frequencies of the reservoir. When the reservoir is in an equilibrium state, it is called a heat bath. The status of the environment is always unknown or not possible to be controlled in reality, therefore it is useful to work with approximation.

Given the density operator  $\rho$  of the total system, the reduced density operator for the subsystem S is obtained by taking the partial trace over the degrees of freedom of the environment B, i.e.  $\rho_S = \operatorname{tr}_{\mathscr{H}_B} \rho$ . As a result, the expectation value of the operator A on the subsystem Hilbert space  $\mathscr{H}_S$  is defined by  $\langle A \rangle = \operatorname{tr}_{\mathscr{H}_S} \{A \rho_S\}$ , and the unitary time evolution for the reduced density operator is in the form

$$\rho_S(t) = \text{tr}_{\mathcal{H}_B} \{ U(t, t_0) \rho(t_0) U^{\dagger}(t, t_0) \}. \tag{75}$$

See more details on open quantum systems in the books of Nielsen [10] and Breuer [11].

## 2.3 Quantum Dynamical Semigroups and Quantum Markovian Master Equations

Let S+B be a total quantum system which is a composite of a reduced system S and an environment B. The state of the total system at the initial time, i.e. t=0, is defined by  $\rho(0) = \rho_S(0) \otimes \rho_B$ . The state of the total system at time t is transformed in terms of the unitary time evolution operator by  $\rho(t) = U(t,0)[\rho_S(0) \otimes \rho_B]U^{\dagger}(t,0)$ . The state of the reduced system at time t is obtained by taking the partial trace of the corresponding total system over the degrees of freedoms of the environment, i.e.

$$\rho_{\mathcal{S}}(t) = \operatorname{tr}_{\mathscr{H}_{\mathcal{B}}} \{ U(t,0) [\rho_{\mathcal{S}}(0) \otimes \rho_{\mathcal{B}}] U^{\dagger}(t,0) \}. \tag{76}$$

Alternatively, we can consider a mapping from  $\rho_S(0)$  to  $\rho_S(t)$ . Note that the states of the reduced system described by the density operators in both initial time  $t_0$  and some fixed time t belong to the same Hilbert space. The mapping is called dynamical map, denoted by  $V(t): \mathcal{S}(\mathcal{H}_S) \mapsto \mathcal{S}(\mathcal{H}_S)$ . As was shown in Breuer's book[11], the full relation can be described by a commutative diagram as follows

$$\rho(0) = \rho_{S}(0) \otimes \rho_{B}^{\text{Unitary time evolution}} \rho(t) = U(t,0) [\rho_{S}(0) \otimes \rho_{B}] U^{\dagger}(t,0)$$

$$\text{tr}_{\mathscr{H}_{B}} \downarrow \qquad \qquad \qquad \downarrow \text{tr}_{\mathscr{H}_{B}}$$

$$\rho_{S}(0) \xrightarrow{\text{Dynamical map}} \rho_{S}(t)$$

The density operator of the environment has a spectral decomposition in the form  $\rho_B = \sum_{\alpha} \lambda_{\alpha} |\phi_{\alpha}\rangle \langle \phi_{\alpha}|$  where  $\sum_{\alpha} \lambda_{\alpha} = 1$  and  $|\phi_{\alpha}\rangle$  is the orthonormal basis for the environment Hilbert space  $\mathscr{H}_B$ . Let us substitute this spectral decomposition into the

equation (76), we obtain the following expression

$$\rho_{S}(t) = \operatorname{tr}_{\mathscr{H}_{B}} \{ U(t,0) [\rho_{S}(0) \otimes (\sum_{\alpha} \lambda_{\alpha} | \phi_{\alpha} \rangle \langle \phi_{\alpha} |)] U^{\dagger}(t,0) \}$$

$$= \sum_{\beta} (I \otimes \langle \phi_{\beta} |) U(t,0) [\rho_{S}(0) \otimes (\sum_{\alpha} \lambda_{\alpha} | \phi_{\alpha} \rangle \langle \phi_{\alpha} |)] U^{\dagger}(t,0) (I \otimes | \phi_{\beta} \rangle)$$

$$= \sum_{\alpha\beta} \sqrt{\lambda_{\alpha}} (I \otimes \langle \phi_{\beta} |) U(t,0) (I \otimes | \phi_{\alpha} \rangle) \rho_{S}(0) \sqrt{\lambda_{\alpha}} (I \otimes \langle \phi_{\alpha} |) U^{\dagger}(t,0) (I \otimes | \phi_{\beta} \rangle)$$

$$= \sum_{\alpha\beta} \sqrt{\lambda_{\alpha}} \langle \phi_{\beta} | U(t,0) | \phi_{\alpha} \rangle \rho_{S}(0) \sqrt{\lambda_{\alpha}} \langle \phi_{\alpha} | U^{\dagger}(t,0) | \phi_{\beta} \rangle$$
(78)

In order to shorten the equation (78), we introduce an operator in the form

$$W_{\alpha\beta}(t) = \sqrt{\lambda_{\alpha}} \langle \phi_{\beta} | U(t) | \phi_{\alpha} \rangle. \tag{79}$$

*Remark.* Since  $\{|\phi\rangle\}$  is an orthonormal basis for the environment Hilbert space  $\mathscr{H}_B$  and U(t) is the operator acting on the total Hilbert space  $\mathscr{H}_S \otimes \mathscr{H}_B$ , thus the Kraus operator is an operator acting on the subsystem Hilbert space  $\mathscr{H}_S$ , as the result of  $\langle \phi_\beta \, | \, U(t) \, | \, \phi_\alpha \rangle = \operatorname{tr}_{\mathscr{H}_B} \left( \, |\phi_\alpha\rangle \, \langle \phi_\beta \, | \, U(t) \, \right)$ .

Then we can rewrite the equation (78) as the operator sum representation as follows

$$V(t)\rho_{S} = \sum_{\alpha\beta} W_{\alpha\beta}(t)\rho_{S}W_{\alpha\beta}^{\dagger}(t). \tag{80}$$

According to the completeness relation, we have  $\sum_{\alpha\beta} W_{\alpha\beta}^{\dagger}(t) W_{\alpha\beta}(t) = I_S$ , and it follows  $\operatorname{tr}_{\mathscr{H}_S} \{V(t)\rho_S\} = \operatorname{tr}_{\mathscr{H}_S} \rho_S = 1$ .

Moreover, this dynamical map has the property  $V(t)(\sum_i \alpha_i \rho_i) = \sum_i \alpha_i V(t) \rho_i$ , where  $p_i \ge 0, \sum_i \alpha_i = 1$ , the property is called convex linearity.

Generally, the dynamical map V(t) is a convex linear, completely positive and trace-preserving map.

The set of all dynamical maps with the variation of time t forms the one-parameter family of the dynamical maps  $\{V(t)|t \geq 0\}$ . The identity map is denoted by V(0). This one-parameter family of the dynamical maps is called quantum dynamical semigroup if it is continuous and equipped with the semigroup property

$$V(t_1)V(t_2) = V(t_1 + t_2), t_1, t_2 > 0.$$
 (81)

Here we mention some definitions from Lindblad's original paper[16].

Let  $\mathscr{A}$  be a  $W^*$ -algebra. An one-parameter family  $\Phi$  of dynamical maps of  $\mathscr{A}$  is a quantum dynamical semigroup if it satisfies

- 1.  $\Phi_t > 0$
- 2.  $\Phi_t(I) = I$
- 3.  $\Phi_s \Phi_t = \Phi_{s+t}$
- 4.  $\Phi_t(X) \mapsto X$  ultraweakly convergent as  $t \mapsto 0$

#### 5. $\Phi_t$ is ultraweakly continuous

*Remark.* The ultraweak continuity of the one-parameter family of the dynamical maps means that we have

$$\lim_{\varepsilon \to 0} \operatorname{tr}_{\mathscr{H}_{S}} \{ (V^{\dagger}(\varepsilon)A - A)\rho_{S} \} = 0, \tag{82}$$

for all  $\rho_S$  and all bounded operators A. The map  $V^{\dagger}(t)$  denotes the Heisenberg picture dynamical map which acts on the bounded operators A such that

$$\operatorname{tr}_{\mathscr{H}_{S}}\{A(V(t)\rho_{S})\} = \operatorname{tr}_{\mathscr{H}_{S}}\{(V^{\dagger}(t)A)\rho_{S}\}$$
(83)

for all  $\rho_S$ .

Let a superoperator  $\mathscr{L}$  be the generator of a quantum dynamical semigroup, the semigroup is represented in the form  $V(t) = \exp(\mathscr{L}t)$ . The dynamics of the reduced density operator is given by  $\frac{d}{dt}\rho_S(t) = \mathscr{L}\rho_S(t)$ .

Let  $\mathcal{H}_S$  be a finite dimensional Hilbert space such that dim  $\mathcal{H}_S = N$ , the corresponding Liouville space is a space consisting of the Hilbert-Schmidt operators. Its dimension is  $N^2$ . We consider the basis of the Liouville space as the orthonormal operators in the form  $F_i$ ,  $i = 1, ..., N^2$  where the inner product is defined by  $(F_i, F_j) = \operatorname{tr}_{\mathcal{H}_S} \{F_i^{\dagger} F_j\} = \delta_{ij}$  where  $\delta_{ij}$  is the Kronecker delta function. For computational simplicity, we assume that in a certain basis, one operator is proportional to the identity matrix, i.e.  $F_{N^2} = \sqrt{\frac{1}{N}} I_S$ , and all others are traceless, i.e.  $\operatorname{tr}_{\mathcal{H}_S} F_i = 0, i = 1, ..., N^2 - 1$ .

According to the completeness relation, the Kraus operator has the form

$$W_{\alpha\beta}(t) = \sum_{i=1}^{N^2} F_i(F_i, W_{\alpha\beta}(t))$$
(84)

and then by substituting it to the equation (80), we have

$$V(t)\rho_{S} = \sum_{\alpha\beta} \left( \sum_{i=1}^{N^{2}} F_{i}(F_{i}, W_{\alpha\beta}(t)) \rho_{S} \sum_{j=1}^{N^{2}} F_{j}^{\dagger}(F_{j}, W_{\alpha\beta}(t))^{*} \right)$$
(85)

$$=\sum_{i,j=1}^{N^2} c_{ij}(t) F_i \rho_S F_j^{\dagger}$$
(86)

where  $c_{ij} = \sum_{\alpha\beta} (F_i, W_{\alpha\beta}(t)) (F_j, W_{\alpha\beta}(t))^*$ .

Let us consider the generator of the quantum dynamical semigroup as the following

form

$$\mathcal{L}\rho_{S} = \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \left( V(\varepsilon) \rho_{S} - \rho_{S} \right) \tag{87}$$

$$= \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \left( \sum_{i,j=1}^{N^{2}} c_{ij}(\varepsilon) F_{i} \rho_{S} F_{j}^{\dagger} - \rho_{S} \right)$$

$$= \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \left( \sum_{i,j=1}^{N^{2}-1} c_{ij}(\varepsilon) F_{i} \rho_{S} F_{j}^{\dagger} + \sum_{i=1,j=N^{2}}^{N^{2}} c_{ij}(\varepsilon) F_{i} \rho_{S} F_{j}^{\dagger} + \sum_{i=N^{2},j=1}^{N^{2}} c_{ij}(\varepsilon) F_{i} \rho_{S} F_{j}^{\dagger} - \sum_{i=N^{2},j=N^{2}}^{N^{2}} c_{ij}(\varepsilon) F_{i} \rho_{S} F_{j}^{\dagger} - \rho_{S} \right)$$

$$= \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \left( \sum_{i,j=1}^{N^{2}-1} c_{ij}(\varepsilon) F_{i} \rho_{S} F_{j}^{\dagger} + \sqrt{\frac{1}{N}} \sum_{i=1}^{N^{2}} c_{iN^{2}}(\varepsilon) F_{i} \rho_{S} + \sqrt{\frac{1}{N}} \sum_{j=1}^{N^{2}} c_{N^{2}j}(\varepsilon) \rho_{S} F_{j}^{\dagger} - \frac{1}{N} c_{N^{2}N^{2}}(\varepsilon) \rho_{S} - \rho_{S} \right)$$

$$= \lim_{\varepsilon \to 0} \frac{1}{\varepsilon} \left\{ \sum_{i,j=1}^{N^{2}-1} c_{ij}(\varepsilon) F_{i} \rho_{S} F_{j}^{\dagger} + \sqrt{\frac{1}{N}} \sum_{i=1}^{N^{2}-1} \left( c_{iN^{2}}(\varepsilon) F_{i} \rho_{S} + c_{N^{2}i}(\varepsilon) \rho_{S} F_{j}^{\dagger} \right) + \frac{1}{N} c_{N^{2}N^{2}}(\varepsilon) \rho_{S} - \rho_{S} \right\}$$

$$= \lim_{\varepsilon \to 0} \left\{ \sum_{i,j=1}^{N^{2}-1} c_{ij}(\varepsilon) F_{i} \rho_{S} F_{j}^{\dagger} + \sqrt{\frac{1}{N}} \sum_{i=1}^{N^{2}-1} \left( c_{iN^{2}}(\varepsilon) F_{i} \rho_{S} + \frac{c_{N^{2}i}(\varepsilon)}{\varepsilon} \rho_{S} F_{j}^{\dagger} \right) + \frac{1}{N} \frac{c_{N^{2}N^{2}}(\varepsilon) - N}{\varepsilon} \rho_{S} \right\}.$$
(88)

In order to shorten the equation (88), we introduce some coeffcients as follows

$$a_{N^2N^2} = \lim_{\varepsilon \to 0} \frac{c_{N^2N^2}(\varepsilon) - N}{\varepsilon} \tag{89}$$

$$a_{iN^2} = \lim_{\varepsilon \to 0} \frac{c_{iN^2}(\varepsilon)}{\varepsilon} \tag{90}$$

$$a_{ij} = \lim_{\varepsilon \to 0} \frac{c_{ij}(\varepsilon)}{\varepsilon} \tag{91}$$

where  $i = 1, ..., N^2 - 1$ , and introduce some operators as follows

$$F = \sqrt{\frac{1}{N}} \sum_{i=1}^{N^2 - 1} a_{iN^2} F_i \tag{92}$$

$$G = \frac{1}{2N} a_{N^2 N^2} I_S + \frac{1}{2} (F^{\dagger} + F)$$
 (93)

$$H = \frac{1}{2i}(F^{\dagger} + F) \tag{94}$$

where H is Hermitian, and  $\sum_{i,j=1}^{N^2-1} a_{ij}$  is a Hermitian matrix. Therefore, we can rewrite the equation (88) as follows

$$\mathcal{L}\rho_{S} = -i[H, \rho_{S}] + \{G, \rho_{S}\} + \sum_{i,j=1}^{N^{2}-1} a_{ij}F_{i}\rho_{S}F_{j}^{\dagger}.$$
 (95)

Due to the trace preserving property of the quantum dynamical semigroup, we have

$$\operatorname{tr}_{\mathscr{H}_{S}}\{\mathscr{L}\rho_{S}\} = 0 = \operatorname{tr}_{\mathscr{H}_{S}}\left\{\left(2G + \sum_{i,j=1}^{N^{2}-1} a_{ij}F_{j}^{\dagger}F_{i}\right)\rho_{S}\right\}$$
(96)

where

$$G = -\frac{1}{2} \sum_{i,j=1}^{N^2 - 1} a_{ij} F_j^{\dagger} F_i. \tag{97}$$

Thus the equation (95) can be rewritten in the form

$$\mathcal{L}\rho_{S} = -i[H, \rho_{S}] + \sum_{i,j=1}^{N^{2}-1} a_{ij} \left( F_{i} \rho_{S} F_{j}^{\dagger} - \frac{1}{2} \left\{ F_{j}^{\dagger} F_{i}, \rho_{S} \right\} \right)$$

$$\tag{98}$$

It is the first standard form of the semigroup generator.

As Breuer showed in his book [11], as the result of positivity of the matrix  $(a_{ij})$ , we can diagonalize it with the aid of the unitary matrix u as follows

$$uau^{\dagger} = \begin{pmatrix} \gamma_1 & 0 & \cdots & 0 \\ 0 & \gamma_2 & \cdots & 0 \\ 0 & 0 & \ddots & 0 \\ 0 & 0 & \cdots & \gamma_{N^2 - 1} \end{pmatrix}. \tag{99}$$

where  $\gamma_i$  are non negative eigenvalues. Let us introduce the operators

$$F_i = \sum_{k=1}^{N^2 - 1} u_{ki} A_k \tag{100}$$

We represent the generator in the diagonal form as follows

$$\mathcal{L}\rho_{S} = -i[H, \rho_{S}] + \sum_{k=1}^{N^{2}-1} \gamma_{k} \left( A_{k} \rho_{S} A_{k}^{\dagger} - \frac{1}{2} A_{k}^{\dagger} A_{k} \rho_{S} - \frac{1}{2} \rho_{S} A_{k}^{\dagger} A_{k} \right). \tag{101}$$

where  $A_k$  are called Lindblad operators.

The equation  $\frac{d}{dt}\rho_S = \mathcal{L}\rho_S$  is usually called Lindblad equation. See also Gorini, Kossakowski and Sudarshan[17].

#### 2.3.1 On (non)Stabilization of the solutions of the von Neumann equation

In this subsection, we study the conditions for stabilization of the solutions of the von Neumann equation.

**Theorem 2.4.** Let the time independent Hamiltonian H be a bounded Hermitian operator. If H commutes with the density matrix at intial time, i.e.  $[H, \rho(0)] = 0$ , then the solution of the von Neumann equation is stabilized at all time scales.

*Proof.* Given  $[H, \rho(0)] = 0$ , we have

$$\frac{d}{dt}\rho(t) = -i[H, U(t,0)\rho(0)U^{\dagger}(t,0)]$$
(102)

$$= -iU(t,0)[H,\rho(0)]U^{\dagger}(t,0)$$

$$= 0$$
(103)

It implies that  $\rho(t) = \rho(0)$  for any time t.

*Remark.* Given  $[H, \rho(0)] = 0$ , we have  $H\rho(0) = \rho(0)H$ . For the corresponding pure states  $|\psi(0)\rangle$ , it follows  $\sum_i w_i H |\psi_i(0)\rangle \langle \psi_i(0)| = \sum_i w_i |\psi_i(0)\rangle \langle \psi_i(0)|H$ . And it implies each of the pure states is the eigenvector of the Hamiltonian H, e.g.  $H |\psi_i(0)\rangle = \lambda |\psi_i(0)\rangle$ .

**Theorem 2.5.** Let the Hamiltonian H be a bounded Hermitian operator. If  $[H, \rho(0)] \neq 0$ , then the solution of the von Neumann equation will never stabilize.

*Proof.* The von Neumann equation has the form

$$\frac{d}{dt}\rho(t) = -ie^{-iHt}[H,\rho(0)]e^{iHt}.$$
(104)

With the aid of the eigenstates (eigenvectors)  $|n\rangle$  of the Hamiltonian, i.e.  $H|n\rangle = E_n|n\rangle$ , where  $E_n$  denotes the energy eigenvalue corresponding to the eigenstate  $|n\rangle$ , we can expand the density matrix as follows:

$$\rho(t) = e^{-iHt} \left( \sum_{m,n} \rho_{mn}(0) |m\rangle \langle n| \right) e^{iHt}$$

$$= \sum_{m,n} \rho_{mn}(0) e^{-iHt} |m\rangle \langle n| e^{iHt}$$

$$= \sum_{m,n} \rho_{mn}(0) e^{-iE_{m}t} |m\rangle \langle n| e^{iE_{n}t}$$

$$= \sum_{m,n} \rho_{mn}(0) e^{-i(E_{m}-E_{n})t} |m\rangle \langle n|$$
(105)

where  $\rho_{mn}(0)$  are the elements in the initial density matrix.

Given the condition that the Hamiltonian does not communte with the initial density matrix, i.e.  $[H, \rho(0)] \neq 0$ , it follows that

$$H\rho(0) = \sum_{m,n} \rho_{mn}(0)H|m\rangle\langle n| = \sum_{m,n} \rho_{mn}(0)E_m|m\rangle\langle n|$$
 (106)

$$\rho(0)H = \sum_{m,n} \rho_{mn}(0) |m\rangle \langle n|H = \sum_{m,n} \rho_{mn}(0) |m\rangle \langle n|E_n.$$
 (107)

For simplification, we assume the spectrum of Hamiltonian H is non-degenerate, i.e.  $E_m \neq E_n$  for  $m \neq n$ , we have the commutator in the form

$$[H, \rho(0)] = H\rho(0) - \rho(0)H = \sum_{m \neq n} (E_m - E_n)\rho_{mn}(0) |m\rangle \langle n|$$
 (108)

where  $(E_m - E_n) \neq 0$  and  $[H, \rho(0)] \neq 0$ . It implies that at least one coefficient  $\rho_{mn}(0)$  with  $m \neq n$  has to be nonzero. The corresponding phase factor in the equation (105) will oscillate forever at the frequency  $E_m - E_n$ .

We conclude that the solution of the von Neumann equation will never stabilize.  $\Box$ 

*Remark.* Theorem 2.4 and Theorem 2.5 show that Schrödinger-von Neumann dynamics cannot be used to model the process of approaching a stationary state from a non-stationary ones. The appearance of oscillating behavior described in 2.5 is one of the reasons to use the theory of open quantum systems based on the Lindblad equation and leading (for some generators) to stabilization regimes.

#### 3 Application to the Quantum Prisoner's Dilemma

The study of optimal strategies in decision theory is called game theory. It started from the works of John von Neumann *Zur Theorie der Gesellschaftsspiele*[20] in 1928.

In this thesis, we deal with a famous game so-called Prisoner's Dilemma. In classical game theory, rational behavior for an individual player is to make a decision which maximizes the player's own payoff. A collection of strategies for players is called a Nash equilibrium if no player will change the chosen strategy, since there is no better strategy when the choices of all other players are fixed. But in reality, there exist irrational behaviors. A statistical experiment by Shafir and Tversky [18], [19] presented that only 63% of the players make rational choices. In the case of the Prisoner's Dilemma, this shows that many people decided to coorperate which is classically considered as an irrational behavior. In order to explain why this probably happens, we introduce a quantum-like decision making model, the so-called Asano-Khrennikov-Ohya model[1], [2], [4], [5].

#### 3.1 Classical 2-player Prisoner's Dilemma

We describe the game "Prisoner's Dillemma" as follows. Suppose there are two criminals, Alice and Bob, who are arrested by the police due to robbery. Then they are separated without being able to communicate. When they are individually investigated by the policeman, they are notified with the following possible consequences: If both of them confess the crime, they will both check in prison for 5 years. If both of them deny the crime, it is 2 years for each. Finally, if one confesses and the other denies, the one who confesses will only serve for 1 year and for 10 years the one who denies.

Each player has two possible strategies, either cooperate denoted by C or defect denoted by D. If they trust each other, they might cooperate, i.e. both deny the crime, in order to obtain the payoffs (C,C)=(2,2) which is good for the group. But they are separated without any communication, and they are both scared to be betrayed, because if one player denies the crime and the other confesses it, the latter will be 10 years in prison, and therefore they both want to betray each other to have the shortest years in prison, i.e. (D,C)=(1,10) and (C,D)=(10,1). This is the rational behavior in classical game theory.

We present the following payoff table

	$C_B$	$D_B$
$C_A$	(2,2)	(10,1)
$D_A$	(1,10)	(5,5)

Then for a more general case: Let a < b < c < d be the payoff, we have the table

$$\begin{array}{c|c} & |C_B\rangle & |D_B\rangle \\ \hline |C_A\rangle & (b,b) & (d,a) \\ \hline |D_A\rangle & (a,d) & (c,c) \\ \end{array}$$

#### 3.1.1 Nash equilibrium

In addition to John von Neumann's works in classical game theory, the papers of John Nash must be mentioned, especially his papers about equilibrium points for non-cooperative games, which is called Nash equilibrium [21], [22].

Let us introduce some basics in classical game theory. An n-player game is a set of n players where each player has a finite set of pure strategies, and each player , i , has a payoff function,  $p_i$ , which maps the set of n-tuples of pure strategies to real numbers. Each entry in the n-tuple refers to a unique single player. A mixed strategy is a convex-linear combination of pure strategies. We define a mixed strategy for a player i to be  $s_i = \sum_{\alpha} c_{i\alpha} \pi_{i\alpha}$  where  $\sum_{\alpha} c_{i\alpha} = 1$  and  $c_{i\alpha} \geq 0$ , and  $\pi_{i\alpha}$  is pure strategy. The payoff function of a player for the mixed strategies is  $p_i(s_1, s_2, \ldots, s_n)$ , where each entry is the mixed strategy for the corresponding player. The n-tuples can be regarded as points in vector space, and the mixed strategy is contained in the product space of vector spaces. In Nash's paper [21], [22], he gave a substitution notation for computational convenience, i.e.  $(\mathbf{s};t_i) = (s_1, s_2, \ldots, s_{i-1}, t_i, s_{i+1}, \ldots, s_n)$ .

The *n*-tuple of strategies is a Nash equilibrium point if and only if for all *i*,

$$p_i(\mathbf{s}) = \max_{\text{all } r_i} [p_i(\mathbf{s}; r_i)]$$
 (109)

An equilibrium point represents an *n*-tuple of mixed strategies for all players which maximizes the payoff for each individual player while the other strategies are fixed. It indicates that every mixed strategy is optimal.

A mixed strategy is a convex-linear combination of pure strategies, we have

$$p_i(\mathbf{s}) = \max_{\text{all } r_i} [p_i(\mathbf{s}; r_i)]$$
$$= \max_{\alpha} [p_i(\mathbf{s}; \pi_{i\alpha})]$$

**Theorem 3.1.** Every finite game has an equilibrium point.

**Theorem 3.2.** Any finite game has a symmetric equilibrium point.

See proofs in Nash's paper[22].

**Example 3.1.** For the Prisoner's Dilemma game, each player's optimal strategy is defect for maximizing her own payoff. The Nash equilibrium is (D, D), and it is unique.

#### 3.2 Quantum 2-player Prisoner's Dilemma: Asano-Khrennikov-Ohya Model

For the Prisoner's Dillemma game, the rational behavior for the players is defect and there exists a unique Nash equilibrium point (D,D). As was pointed, the players can demonstrate irrational behavior by selecting strategies different from the Nash equilibrium. In this section, we introduce the Asano-Khrennikov-Ohya model[1], [2], [4], [5] for a possible explanation why irrational behavior happens.

Given a player A, she doesn't know anything about which decision the player B will make, but she may guess. We consider it as a quantum superposition state on the

Hilbert space  $\mathscr{H} = \mathbb{C}^2$ , named prediction state and denoted by  $|\phi_B\rangle = \alpha |0_B\rangle + \beta |1_B\rangle$  where  $|\alpha|^2 + |\beta|^2 = 1$ . We call  $\{|0_B\rangle, |1_B\rangle\}$  the prediction basis.

The player A can choose either 0 or 1. These choices are represented by the decision basis  $\{|0_A\rangle, |1_A\rangle\}$ . Coupled with the prediction state for the player B, there will be two consequences which is also in a quantum superposition state, called alternative state and denoted by  $|\Phi_0\rangle = \alpha |0_A 0_B\rangle + \beta |0_A 1_B\rangle = |0_A\rangle \otimes |\phi_B\rangle$  if she chooses 0, and  $|\Phi_1\rangle = \alpha |1_A 0_B\rangle + \beta |1_A 1_B\rangle = |1_A\rangle \otimes |\phi_B\rangle$  for choosing 1.

With two alternative states, there is a new quantum superposition state, called mental state, dentoed by  $|\Psi\rangle=x|\Phi_0\rangle+y|\Phi_1\rangle$ . Formally (in the operational framework), this state can be treated as the state of a composite quantum system, i.e.  $\mathbb{C}^2\otimes\mathbb{C}^2$ . The corresponding operator of the mental state is defined by

$$|\Psi\rangle\langle\Psi| = |x|^2 |\Psi_0\rangle |\Psi_0\rangle + |y|^2 |\Psi_1\rangle |\Psi_1\rangle + xy^* |\Psi_0\rangle |\Psi_1\rangle + yx^* |\Psi_1\rangle |\Psi_0\rangle, \quad (110)$$

which has the corresponding density matrix in the form  $\rho_{\Psi} = \begin{pmatrix} |x|^2 & xy^* \\ yx^* & |y|^2 \end{pmatrix}$ .

An important idea of the model is that the decision maker is a self-observer which enables the player to guess the other's decision. Therefore, the player's own mind is considered as an open quantum system. The self-imaging of the prediction for the other's decision is regarded as the environment which is also a quantum system, since the decision maker can generate a mental reservoir by itself. We consider the interaction as being between the player's own decision and the mental self-image of the other's decision.

The dynamics in an open quantum system is described by the Lindblad equation (101). By choosing a specific Lindblad operator which provides a stabilized solution, it can lead the density matrix to an equilibrium state. One can say it is the termination of the comparison process for a decision maker. This equilibrium density matrix describes a mixed strategy, where we can get the probability for each corresponding pure strategy by making a quantum measurement. (See equations (140) and (141))

#### 3.2.1 Examples of Lindblad Equations

In this section, we present some examples of the Lindblad equation.

**Example 3.2.** Let us consider a two level atom for the spontaneous emission, and let us assume the ground state is  $|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ , the exicited state is  $|1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ , and the Hamiltonian is  $H = -\frac{\omega_0}{2}\sigma_z$  where  $\sigma_z$  is the Pauli matrix and  $\omega_0$  is the energy difference between the ground state and excited state. Then let us assume the Lindblad operator  $A = \sqrt{\Gamma} \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$  which indicates the relaxation process from  $|1\rangle$  to  $|0\rangle$ . Therefore, we have the corresponding Lindblad equation

$$\frac{\partial}{\partial t} \begin{pmatrix} \rho_{00} & \rho_{01} \\ \rho_{10} & \rho_{11} \end{pmatrix} = -i[H, \rho] + A\rho A^{\dagger} - \frac{1}{2}(A^{\dagger}A\rho + \rho A^{\dagger}A)$$
(111)

$$= i\omega_0 \begin{pmatrix} 0 & \rho_{01} \\ -\rho_{10} & 0 \end{pmatrix} + \Gamma \begin{pmatrix} \rho_{11} & -\frac{1}{2}\rho_{01} \\ -\frac{1}{2}\rho_{10} & -\rho_{11} \end{pmatrix}. \tag{112}$$

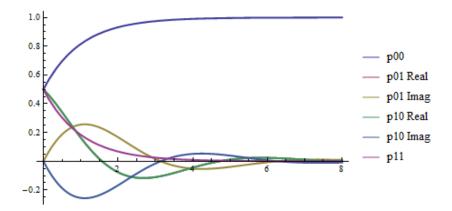


Figure 1: Solutions of Lindblad equation for spotaneous emission

The analytic solution has the form

$$\rho_{00}(t) = \rho_{00}(0) + \rho_{11}(0)(1 - \exp(-\Gamma t))$$
(113)

$$\rho_{01}(t) = \rho_{01}(0) \exp(i\omega_0 t - \frac{\Gamma}{2}t)$$
(114)

$$\rho_{10}(t) = \rho_{10}(0) \exp\left(-i\omega_0 t - \frac{\Gamma}{2}t\right)$$
 (115)

$$\rho_{11}(t) = \rho_{11}(0) \exp(-\Gamma t). \tag{116}$$

*Remark.* Given  $\frac{d}{dt}\rho_{00}(t) = \Gamma\rho_{11}(t)$ , it implies  $\rho_{00}(t) = C - \rho_{11}(0) \exp(-\Gamma t)$ . We can find  $C = \rho_{00}(0) + \rho_{11}(0)$ . By substituting it back, we obtain the equation (113).

We assume  $\omega_0 = \Gamma_+ = \Gamma_- = \Gamma_z = 1$  for the computational simplicity. With the assumed symmetric initial condition  $\rho(0) = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} \otimes (\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}})$ , we present the graph for the solutions as  $t \to \infty$  in the Figure 1.

Analytically, we can prove  $\rho(t)$  is a diagonal matrix as  $t \to \infty$  as follows

$$\lim_{t \to \infty} \rho_{01}(t) = \lim_{t \to \infty} \left( \rho_{01}(0) \frac{\cos(\omega_0 t)}{e^{\frac{\Gamma}{2}t}} + \rho_{01}(0) i \frac{\sin(\omega_0 t)}{e^{\frac{\Gamma}{2}t}} \right) = 0$$
 (117)

$$\lim_{t \to \infty} \rho_{10}(t) = \lim_{t \to \infty} \left( \rho_{10}(0) \frac{\cos(\omega_0 t)}{e^{\frac{\Gamma}{2}t}} - \rho_{10}(0) i \frac{\sin(\omega_0 t)}{e^{\frac{\Gamma}{2}t}} \right) = 0.$$
 (118)

We present the graph of the von Neumann entropy for the density matrix in the Figure 2.

*Remark.* Note that the von Neumann entropy is decreasing to 0 with as  $t \to \infty$ . Additionally, one of the diagonal entry in the density matrix tends to 0 which means the limiting density matrix describes the pure states. This situation will happen again in the Example 3.4.

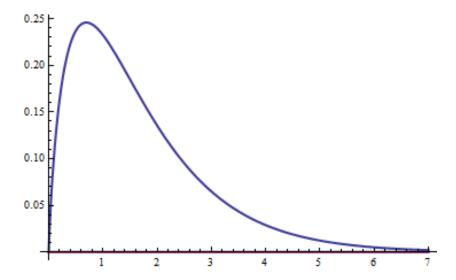


Figure 2: von Neumann entropy of the density matrix for spotaneous emission

**Example 3.3.** Let us consider the Bloch equation in Nuclear Magnetic Resonance (NMR) and we assume the Hamiltonian is  $H=-\frac{\omega_0}{2}\sigma_z$ , and three Lindblad operators are  $A_+=\sqrt{\Gamma_+}\begin{pmatrix}0&1\\0&0\end{pmatrix}$ ,  $A_-=\sqrt{\Gamma_-}\begin{pmatrix}0&0\\1&0\end{pmatrix}$  and  $A_z=\sqrt{\Gamma_z}\begin{pmatrix}1&0\\0&-1\end{pmatrix}$  where  $A_+$  is the relaxation process from the excited state to the ground state,  $A_-$  is the exictation process from the ground state to the exited state and  $A_z$  is the dephasing process such that there is no energy transmission for the spin with the environment.

We present the corresponding Linblad equation

$$\frac{\partial}{\partial t} \begin{pmatrix} \rho_{00} & \rho_{01} \\ \rho_{10} & \rho_{11} \end{pmatrix} = i\omega_0 \begin{pmatrix} 0 & \rho_{01} \\ -\rho_{10} & 0 \end{pmatrix} + \Gamma_+ \begin{pmatrix} \rho_{11} & -\frac{1}{2}\rho_{01} \\ -\frac{1}{2}\rho_{10} & -\rho_{11} \end{pmatrix} + \Gamma_- \begin{pmatrix} -\rho_{00} & -\frac{1}{2}\rho_{01} \\ -\frac{1}{2}\rho_{10} & \rho_{00} \end{pmatrix} + \Gamma_z \begin{pmatrix} 0 & -2\rho_{01} \\ -2\rho_{10} & 0 \end{pmatrix}.$$
(119)

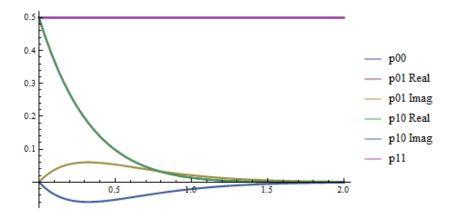


Figure 3: Solutions of Lindblad equation for Bloch equation in NMR with symmetric initial condition

The analytic solution has the form

$$\rho_{00}(t) = \rho_{00}(0) \frac{\exp(-(\Gamma_{+} + \Gamma_{-})t)\Gamma_{-} + \Gamma_{+}}{\Gamma_{+} + \Gamma_{-}} - \rho_{11}(0) \frac{\exp(-(\Gamma_{+} + \Gamma_{-})t)\Gamma_{+} - \Gamma_{+}}{\Gamma_{+} + \Gamma_{-}}$$

(120)

$$\rho_{01}(t) = \rho_{01}(0) \exp((i\omega_0 - \frac{\Gamma_+}{2} - \frac{\Gamma_-}{2} - 2\Gamma_z)t)$$
(121)

$$\rho_{10}(t) = \rho_{10}(0) \exp((-i\omega_0 - \frac{\Gamma_+}{2} - \frac{\Gamma_-}{2} - 2\Gamma_z)t)$$
(122)

$$\rho_{11}(t) = \rho_{00}(0) \frac{-\exp(-(\Gamma_{+} + \Gamma_{-})t)\Gamma_{-} + \Gamma_{-}}{\Gamma_{+} + \Gamma_{-}} + \rho_{11}(0) \frac{\exp(-(\Gamma_{+} + \Gamma_{-})t)\Gamma_{+} + \Gamma_{-}}{\Gamma_{+} + \Gamma_{-}}.$$
(123)

We assume  $\omega_0=\Gamma_+=\Gamma_-=\Gamma_z=1$  for the computational simplicity. With the assumed symmetric initial condition  $\rho(0)=\begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix}$ , we present the graph for the solutions as  $t\to\infty$  in the Figure 3. , and for the asymmetric initial condition  $\rho(0)=\begin{pmatrix} \frac{1}{3} & \frac{\sqrt{2}}{3} \\ \frac{\sqrt{2}}{3} & \frac{2}{3} \end{pmatrix}=\begin{pmatrix} \frac{1}{\sqrt{3}} \\ \frac{\sqrt{2}}{\sqrt{3}} \end{pmatrix}\otimes (\frac{1}{\sqrt{3}},\frac{\sqrt{2}}{\sqrt{3}})$  in the Figure 4.

*Remark*. We present an analytic proof that the  $\rho_{00}$ ,  $\rho_{11}$  are approaching to the same limit when it has the asymmetric initial condition as  $t \to \infty$ . Let us substitute the

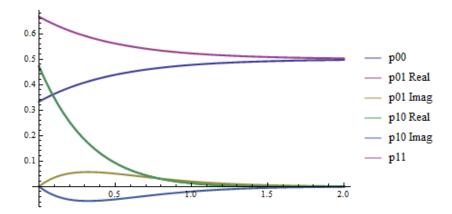


Figure 4: Solutions of Lindblad equation for Bloch equation in NMR with asymmetric initial condition

asymmetric initial condition into the equation (120) and equation (123), we have

$$\lim_{t \to \infty} \rho_{00}(t) = \frac{1}{2} - \frac{e^{-2t}}{6} = \frac{1}{2}$$
 (124)

$$\lim_{t \to \infty} \rho_{11}(t) = \frac{1}{2} + \frac{e^{-2t}}{6} = \frac{1}{2}$$
 (125)

(126)

It is proven that  $\rho_{00}$  and  $\rho_{11}$  are approaching the same limit at 0.5 as  $t \to \infty$ . Analytically, we can prove  $\rho(t)$  is a diagonal matrix as  $t \to \infty$  as follows

$$\lim_{t \to \infty} \rho_{01}(t) = \lim_{t \to \infty} \left( \rho_{01}(0) \frac{\cos(\omega_0 t)}{e^{(\frac{\Gamma_+}{2} + \frac{\Gamma_-}{2} + 2\Gamma_z)t}} + \rho_{01}(0) i \frac{\sin(\omega_0 t)}{e^{(\frac{\Gamma_+}{2} + \frac{\Gamma_-}{2} + 2\Gamma_z)t}} \right) = 0$$
 (127)

$$\lim_{t \to \infty} \rho_{10}(t) = \lim_{t \to \infty} \left( \rho_{10}(0) \frac{\cos(\omega_0 t)}{e^{(\frac{\Gamma_+}{2} + \frac{\Gamma_-}{2} + 2\Gamma_z)t}} - \rho_{10}(0) i \frac{\sin(\omega_0 t)}{e^{(\frac{\Gamma_+}{2} + \frac{\Gamma_-}{2} + 2\Gamma_z)t}} \right) = 0.$$
 (128)

We present the graph of the von Neumann entropy for the density matrix in the Figure 5

*Remark.* Note that the von Neumann entropy increases and being convergent after some time. This is because  $\rho_{00}$  and  $\rho_{11}$  are approaching to the same limit and stable after some time. Therefore, the limiting density matrix describes the quantum system in a mixed state. Since the probabilities for  $\rho_{00}$  and  $\rho_{11}$  are the same with 50%. According to our cognitive model (See section 3.2), the player has the same probability of either choosing 0 or choosing 1. Probabilistically, each of the decisions can be made by the player.

**Example 3.4.** Let us assume the Hamiltonian is  $H = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$  and Lindblad operator

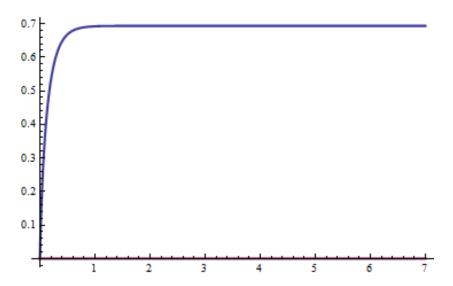


Figure 5: von Neumann entropy of the density matrix for Bloch equation

is  $A = \begin{pmatrix} 0 & i \\ 0 & 0 \end{pmatrix}$ , then we can write the corresponding Lindblad equation

$$\frac{\partial}{\partial t} \begin{pmatrix} \rho_{00} & \rho_{01} \\ \rho_{10} & \rho_{11} \end{pmatrix} = -i[H, \rho] + A\rho A^{\dagger} - \frac{1}{2} (A^{\dagger} A \rho + \rho A^{\dagger} A) \tag{129}$$

$$= -i \left\{ \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \rho - \rho \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \right\} + \begin{pmatrix} 0 & i \\ 0 & 0 \end{pmatrix} \rho \begin{pmatrix} 0 & 0 \\ -i & 0 \end{pmatrix}$$

$$-\frac{1}{2} \left\{ \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \rho + \rho \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} \right\}$$

$$= \begin{pmatrix} \rho_{11} & -\frac{1}{2} \rho_{01} \\ -\frac{1}{2} \rho_{10} & -\rho_{11} \end{pmatrix}$$
(131)

The analytic solution has the form

$$\rho_{00}(t) = \rho_{00}(0) + \rho_{11}(0) - \rho_{11}(0) \exp(-t)$$
(132)

$$\rho_{01}(t) = \rho_{01}(0) \exp(-\frac{1}{2}t)$$
(133)

$$\rho_{10}(t) = \rho_{10}(0) \exp(-\frac{1}{2}t) \tag{134}$$

$$\rho_{11}(t) = \rho_{11}(0) \exp(-t). \tag{135}$$

With the assumed symmetric initial condition  $\rho(0)=\begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix}$ , we present the graph for the solutions as  $t\to\infty$  in the Figure 6.

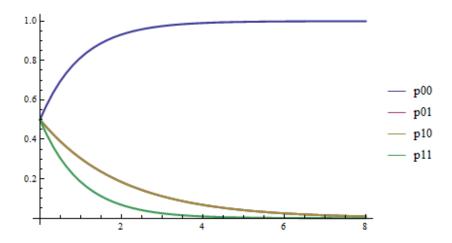


Figure 6: Solutions of Lindblad equation

Analytically, we can prove  $\rho(t)$  is a diagonal matrix as  $t \to \infty$  as follows

$$\lim_{t \to \infty} \rho_{01}(t) = \lim_{t \to \infty} \left( \rho_{01}(0) \frac{1}{\rho_2^{\frac{1}{2}t}} \right) = 0$$
 (136)

$$\lim_{t \to \infty} \rho_{10}(t) = \lim_{t \to \infty} \left( \rho_{10}(0) \frac{1}{\rho_2^{\frac{1}{2}t}} \right) = 0.$$
 (137)

We present the graph of the von Neumann entropy for the density matrix in the Figure 7

*Remark.* Note that the von Neumann entropy increases at the beginning since the non-diagonal entries vanished slower than the diagonal entries. But after some time, the final behavior is that all entries except  $\rho_{00}$  decreases to 0. Therefore, the limiting density matrix describes the quantum system in a pure state.

**Example 3.5.** Let us assume the Hamiltonian is  $H = \tau \sigma_x$  where  $\tau > 0$  and  $\sigma_x$  is a Pauli matrix  $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ , and the Linblad operator is  $A = \tau \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$ . Then we write the corresponding Lindblad equation

$$\frac{\partial}{\partial t} \begin{pmatrix} \rho_{00} & \rho_{01} \\ \rho_{10} & \rho_{11} \end{pmatrix} = -i[H, \rho] + A\rho A^{\dagger} - \frac{1}{2}(A^{\dagger}A\rho + \rho A^{\dagger}A) \tag{138}$$

$$= -\tau i \begin{pmatrix} \rho_{10} - \rho_{01} & \rho_{11} - \rho_{00} \\ \rho_{00} - \rho_{11} & \rho_{01} - \rho_{10} \end{pmatrix} + \tau^2 \begin{pmatrix} \rho_{11} & -\frac{1}{2}\rho_{01} \\ -\frac{1}{2}\rho_{10} & -\rho_{11} \end{pmatrix}$$
(139)

Note that the analytic solutions are too complicated to deal with, then it is better to present the numerical solutions and the von Neumann entropy is still possible to be calculated numerically.

With the assumed symmetric initial condition  $\rho(0) = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix}$ , we present the graph for the solutions as  $t \to \infty$  in the Figure 8.

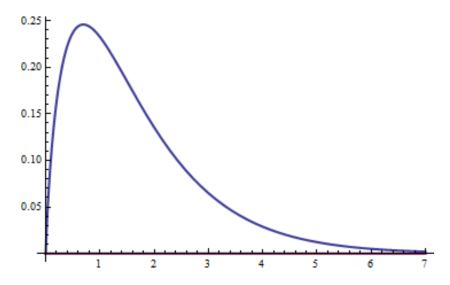


Figure 7: von Neumann entropy of the density matrix

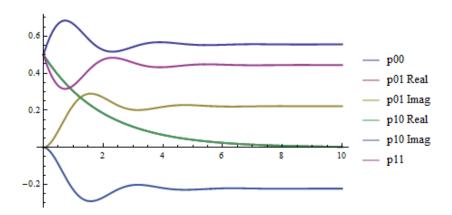


Figure 8: Solutions of Lindblad equation

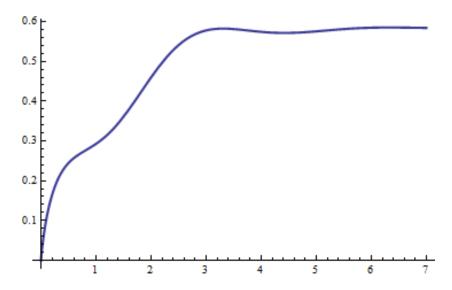


Figure 9: von Neumann entropy of the density matrix

We present the graph of the von Neumann entropy for the density matrix in the Figure 9

*Remark.* Note that the von Neumann entropy increases, it means the limiting density matrix describes the quantum system in a mixed state, as is shown in the Figure 9. In our cognitive model, we can consider the corresponding pure state with the higher probability after a quantum measurement will refer to the decision of the player.

#### 3.2.2 Quantum Decoherence and Quantum Darwinism

For an open quantum system, quantum decoherence leads to collapse of the wave function. The coherence of superpositions has a very short decay time scale. In the Copenhagen interpretation of quantum mechanics, the wave function collapse leads to observations of pure states probabilistically. In addition, it provides a process of selecting pointer base. In quantum mechanics, it is still an open problem how the wave function collapse really happens which is called the measurement problem. It is infeasible to observe internally, therefore many different interpretations of quantum mechanics are provided.

A canonical example is a thought experiment called Schrödinger's Cat such that there are a cat, a glass of poisonous gas and a radioactive switch for the glass in an isolated box. If a single atom decay is detected, then the radioactive switch will be opened and the poisonuous gas will be released. As a result, the cat will be killed. According to the Copenhagen interpretation, after some time, the cat will be in a quantum superposition of two pure states, i.e. alive and dead. Due to quantum decoherence, the cat will not persist forever in superposition. Regarding the observation of a cat in our classical world: it can only be either alive or dead, but not both. Then the question is,

when and how exactly the quantum superposition is destroyed, i.e. the wave function collapses, where the time evolution of quantum state vectors is driven by Schrödinger equations.

W. Zurek proposed[40] that the process of selecting quantum states which leads to the stabilization of the pointer states is analogous to Darwinian natural selection. It provides a possible explanation for the emergence of observations in the classical world from the quantum world. This is called Quantum Darwinism.

In an open quantum system, a selection process so-called einselection (Environment-induced superselection) transforms the superpositions of a quantum system to a reduced set of the pointer states, and the preferred basis after decoherence is the pointer basis which interprets the classical observation.

These pointer states are selected in a way analogous to the Darwinian natural selection. Let us introduce the Darwinian algorithm as follows

- 1. Reproduction: Implementing copies to generate descendants.
- 2. Selection: For the enriched trait in the population after generations, it is preferred to be selected over other traits.
- 3. Variation: Herited trait difference affecting the potential to survive

Analogously, we present the Quantum Darwinism as follows

- 1. Copies consisting of pointer states
- 2. Evolution of pointer states is continuous and predictable such that the trait inheritance for the descendants is from ancestor states.
- 3. Environmental interactions provide evolution and the survived states correspond to the predictable observations in the classical world.

In our quantum-like decision making model, we expect the player's final decision to be made by a quantum measurement on the pointer basis, where the quantum decoherence leads to stabilization of the density matrix which is evolved by the Lindblad equation.

When the density matrix is stabilized at an equilibrium state and being diagonal in the limit as  $t \to \infty$ , we can consider the comparison process in the player's mental dynamics as terminated. In this ideal mathematical model, the non-diagonal elements approach zero only in the limit  $t \to \infty$ . This situation physically and psychologically corresponds to the presence of two time scales determined by the process of decision making, the very fine time scale of mental dynamics and the rough time scale of conscious decision making, respectively. Then the final decision is made probabilistically by performing a quantum measurement as follows

$$|\Phi_0|^2 = \operatorname{tr}\{|0_A\rangle\langle 0_A | \rho_{out} | 0_A\rangle\langle 0_A |\}$$
(140)

$$|\Phi_1|^2 = \operatorname{tr}\{|1_A\rangle\langle 1_A|\rho_{out}|1_A\rangle\langle 1_A|\},\tag{141}$$

where  $|\Phi_0|^2$ ,  $|\Phi_1|^2$  are the probabilities for choosing 0 and 1, respectively.

Additionally, the mental dynamics in the comparison process can explain why there are irrational behaviors.

Now let us reformulate the presented examples of the Lindblad equation in the last chapter as a system of linear differential equations and explain the meaning to our corrsponding cognitive models.

For the example 3.2, we present the system of differential equations

$$\frac{\partial}{\partial t}\rho_{00}(t) = \Gamma \rho_{11}(t) \tag{142}$$

$$\frac{\partial}{\partial t}\rho_{01}(t) = (i\omega_0 - \frac{\Gamma}{2})\rho_{01}(t) \tag{143}$$

$$\frac{\partial}{\partial t}\rho_{10}(t) = (-i\omega_0 - \frac{\Gamma}{2})\rho_{10}(t) \tag{144}$$

$$\frac{\partial}{\partial t}\rho_{11}(t) = -\Gamma\rho_{11}(t) \tag{145}$$

and the limiting density matrix

$$\lim_{t \to \infty} \begin{pmatrix} \rho_{00}(t) & \rho_{01}(t) \\ \rho_{10}(t) & \rho_{11}(t) \end{pmatrix} = \begin{pmatrix} \rho_{00}(0) + \rho_{11}(0) & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$
(146)

In this system of differential equations with the initial conditions, as shown in the section of examples, the corresponding probability for  $\rho_{11}$  will decrease to 0, and the corresponding probability for  $\rho_{00}$  will increase, where the speed slows down when time t increases. For  $\rho_{01}$ ,  $\rho_{10}$ , their imaginary parts will fluctuate at the beginning and stabilize after some time t. Their real parts will decrease to 0 with respect to time t. This dynamical process is shown in the Figure 1, and it can be regarded as the player's mental dynamics for the comparison process of all possible consequences. In the last part of the example 3.2, we have proven that  $\rho(t)$  will be a diagonal matrix as  $t \to \infty$ . As is shown in the equation (146), the limiting density matrix is describing the pure state. When we consider the comparison process is terminated, we can see that after performing the quantum measurement by applying the equation (140) and the equation (141), the player will have 100% to make the decision corresponding to the choice 0 and 0% for the decision corresponding to the choice 1.

For the example 3.3, we present the system of differential equations

$$\frac{\partial}{\partial t}\rho_{00}(t) = -\Gamma_{-}\rho_{00}(t) + \Gamma_{+}\rho_{11}(t) \tag{147}$$

$$\frac{\partial}{\partial t} \rho_{01}(t) = (i\omega_0 - \frac{\Gamma_+}{2} - \frac{\Gamma_-}{2} - 2\Gamma_z)\rho_{01}(t)$$
 (148)

$$\frac{\partial}{\partial t}\rho_{10}(t) = \left(-i\omega_0 - \frac{\Gamma_+}{2} - \frac{\Gamma_-}{2} - 2\Gamma_z\right)\rho_{10}(t) \tag{149}$$

$$\frac{\partial}{\partial t}\rho_{11}(t) = \Gamma_{-}\rho_{00}(t) - \Gamma_{+}\rho_{11}(t) \tag{150}$$

and the limiting density matrix

$$\lim_{t \to \infty} \begin{pmatrix} \rho_{00}(t) & \rho_{01}(t) \\ \rho_{10}(t) & \rho_{11}(t) \end{pmatrix} = \begin{pmatrix} \frac{\rho_{00}(0) + \rho_{11}(0)}{2} & 0 \\ 0 & \frac{\rho_{00}(0) + \rho_{11}(0)}{2} \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{pmatrix}$$
(151)

In this system of differential equations with the initial conditions as is shown in the section of examples, the corresponding probabilities for  $\rho_{00}$  and  $\rho_{11}$  are analogous to the chemical equilibrium. The increment of the corresponding probability for  $\rho_{00}$  is proportional to the value of  $\rho_{11}$  and for  $\rho_{11}$  it is inversely proportional to the value of  $\rho_{00}$  respect to the time t. This will finally lead to an equilibrium. For  $\rho_{01}$ ,  $\rho_{10}$ , their imaginary parts will fluctuate at the beginning and stabilize after some time t and their real parts will decrease to 0 with respect to the time t. This dynamical process is shown in Figure 4 and it can be regarded as the player's mental dynamics for the comparison process of all possible consequences. In the last part of Example 3.3, we have proven that  $\rho(t)$  will be a diagonal matrix as  $t \to \infty$ . As is shown in the equation (151), the limiting density matrix is describing the mixed state. When we consider the comparison process is terminated, we can see that after performing the quantum measurement by applying the equation (140) and the equation (141), the player will have 50% to make the decision corresponding to the choice 0 and 50% for the decision corresponding to the choice 1.

For the Example 3.4, we present the system of differential equations

$$\frac{\partial}{\partial t}\rho_{00}(t) = \rho_{11}(t) \tag{152}$$

$$\frac{\partial}{\partial t}\rho_{01}(t) = -\frac{1}{2}\rho_{01}(t) \tag{153}$$

$$\frac{\partial}{\partial t}\rho_{10}(t) = -\frac{1}{2}\rho_{10}(t) \tag{154}$$

$$\frac{\partial}{\partial t}\rho_{11}(t) = -\rho_{11}(t) \tag{155}$$

and the limiting density matrix

$$\lim_{t \to \infty} \begin{pmatrix} \rho_{00}(t) & \rho_{01}(t) \\ \rho_{10}(t) & \rho_{11}(t) \end{pmatrix} = \begin{pmatrix} \rho_{00}(0) + \rho_{11}(0) & 0 \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$
(156)

The situation for this example is similar to that of Example 3.2.

For the example 3.5, we present the system of differential equations

$$\frac{\partial}{\partial t}\rho_{00}(t) = \tau i \rho_{01}(t) - \tau i \rho_{10}(t) + \tau^2 \rho_{11}(t)$$
(157)

$$\frac{\partial}{\partial t}\rho_{01}(t) = \tau i\rho_{00}(t) - \frac{\tau^2}{2}\rho_{01}(t) - \tau i\rho_{11}(t)$$
(158)

$$\frac{\partial}{\partial t}\rho_{10}(t) = -\tau i\rho_{00}(t) - \frac{\tau^2}{2}\rho_{10}(t) + \tau i\rho_{11}(t)$$
(159)

$$\frac{\partial}{\partial t}\rho_{11}(t) = -\tau i\rho_{01}(t) + \tau i\rho_{10}(t) - \tau^2\rho_{11}(t)$$
(160)

and the approximated limiting density matrix from the numerical simulation with the symmetric initial condition (since we do not have the analytic solution)

nmetric initial condition (since we do not have the analytic solution)
$$\lim_{t \to \infty} \begin{pmatrix} \rho_{00}(t) & \rho_{01}(t) \\ \rho_{10}(t) & \rho_{11}(t) \end{pmatrix} \approx \begin{pmatrix} 0.555294 & 0.0055545 + 0.222162i \\ 0.0055545 - 0.222162i & 0.444706 \end{pmatrix}$$
(161)

In this system of differential equations with the initial conditions as shown in the section of examples, for the real part, the behavior is similar to that of Example 3.2 and Example 3.4. For the imaginary parts of each one, there will be fluctuation at the beginning and they stabilize after some time t. This dynamical process is shown in Figure 8 and it can be regarded as the player's mental dynamics for the comparison process of all possible consequences. Since the analytic solution for this system is too complicated to deal with, we can refer to a graphically numerical solutions to predict the dynamical behaviors. As is shown in the equation (161), the limiting density matrix is describing the mixed state. When we consider the comparison process as terminated, we can see that after performing a quantum measurement by applying equation (140) and equation (141), the player will approximately have 56% to make the decision corresponding to the choice 0 and 44% for the decision corresponding to the choice 1.

*Remark.* The decision making process is closely related to quantum decoherence where a stabilized solution is required. Therefore, not all Lindblad operators will be useful in general. For an equilibrium state of the mental dynamics, we need a Lindblad equation with a stabilizable solution.

#### 4 Conclusion

The aim of this thesis is to numerically simulate and analyze a decision making model proposed by Asano, Khrennikov and Ohya [1]-[6]. The model is based on the representation of mental information processing with the aid of the mathematical formalism of the theory of open quantum systems. For the Prisoner's Dilemma game, we model the processes of decision making by using a Lindblad equation to describe the dynamics of players' mental state("belief-state"). With several numerical simulations, we present both graphically and analytically the stabilized solutions together with the von Neumann entropies. Then we discuss the meaning of the stabilized solutions and the behavior of the von Neumann entropies in the context of cognitive dynamics, and how the decisions are made by the player.

Initially, we present a detailed derivation of the Lindblad equation followed by several examples which we solve both analytically and numerically, and we also present the corresponding dynamics of the von Neumann entropy. In addition, as the main analytical part of this thesis, we prove two theorems about the (non)stabilization of the solution of the von Neumann equation.

Then we illustrate the application of the Asano-Khrennikov-Ohya decision making model for the game of the Prisoner's Dilemma by using the result of numerical and analytical studies of the solutions of concrete Lindblad equations. We note that a decision maker is considered as a self-observer such that she can guess the other's decisions. Both her own decision and her guess of the other's decisions are supposed to be in quantum superpositions. The quantum system of the self-imaging of guessing the other's decisions can be treated as an environment, i.e. mental reservoir. Such a mental reservoir can be generated by itself, and the (information)interaction is between the own decision and the mental self-image of possible actions of the other player. This information structure is regarded as an open quantum system(information). The dynamics in this open quantum system is described by the Lindblad equation, and a

specific Lindblad operator will be useful only if it provides stabilization of solutions. When the quantum decoherence leads to an equilibrium state, it is considered as the termination of the comparison process by the player. Then the player's pure strategy can be selected probabilistically by performing a quantum measurement in the pointer basis. Such quantum decoherence is crucial and essential for the decision making process.

In classical game theory, the rational behavior of a player is to select the strategies corresponding to a Nash equilibrium. Specifically, in the Prisoner's Dilemma, the behavior of a player is considered as rational if she decides to betray. But in real experiments in cognitive psychology which were performed by Tversky and Shafir [18], [19], the statistical data show that there exists irrational behavior. One of the possible methods to explain why it probably happens is to use the mathematical apparatus of QM to model the mental dynamics of a player. This model is referred to the Asano-Khrennikov-Ohya decision making model.

We remark that the model in this thesis is only based on the mathematical apparatus of QM, rather than the real quantum physical model. In fact, not only do we not present any relation to the neural basis for the Asano-Khrennikov-Ohya model, but also it is still an unsolved problem whether or not there really exists quantum phenomenon in the human brains. Such an argument started decades ago but still continues at present time. We refer to the works by Penrose and Hameroff[23]-[27] who are considered as the representative supporters for the quantum brain theory. In their Orch-OR (Orchestrated Objective Reduction) model, they claim that the consciousness is generated by quantum gravity effects in the microtubules. As an opponent, Tegmark[77] argued that according to the calculation, the time scale for the neuron to fire a spike and being excited in the microtubules is much smaller than the decoherence time. However, we emphasize once again that the study in this thesis has not any direct relation to quantum physical models of brain's functioning. The model under analysis is a purely informational model which is based on the assumption (confirmed by the experimental data from cognitive psychology) that information processing performed by complex cognitive systems can be modelled by using the mathematical formalism of the theory of open quantum systems.

## 5 Further works and frontiers in Theoretical Neuroscience

In this thesis, we derived the Lindblad equation for a class of open quantum systems from the Liouville-von Neumann equation, and presented its application to quantum-like decision making process for a 2-player prisoner's dilemma by using the Asano-Khrennikov-Ohya model [1], [2], [4], [5]. As a continuation, the 3-player case will be studied in further works.

In quantum neural computation, Ivancevic has published a book [36] which presents a model to describe the dynamics of quantum microtubules by using a Liouville-von Neumann equations. It will be interesting to discuss the microtubules dynamics in the context of an open quantum system by applying Lindblad equations.

In computational neuroscience [38], [39], a paper published by Cowan [35] introduced a Neural Network Master Equation to describe stochastic neural networks. He presented the transition rates between the neural states as  $|0\rangle \rightarrow |1\rangle$  and  $|1\rangle \rightarrow |0\rangle$ . It follows a configuration of the neural network as the direct product space of all the neural states, i.e.  $|\Omega\rangle = |v_1\rangle |v_2\rangle \dots |v_N\rangle$  where  $v_i \in \{0,1\}$ . This provides a neural network state

$$|\Psi(t)\rangle = \sum_{\Omega} P(\Omega, t) |\Omega\rangle,$$
 (162)

where  $P(\Omega,t)$  is the probability of a certain state  $\Omega$  at the time t. Then the neural network master equation is in the form

$$-\frac{\partial}{\partial t}|\Psi(t)\rangle = \mathcal{L}|\Psi(t)\rangle, \qquad (163)$$

where  $\mathscr{L}$  is the Liouville operator denoted by

$$\mathcal{L} = \alpha \sum_{i=1}^{N} (\sigma_i^+ - 1) \sigma_i^- + \sum_{i=1}^{N} (\sigma_i^- - 1) \sigma_i^+ \phi (\frac{1}{n} \sum_{j=1}^{N} w_{ij} \sigma_j^+ \sigma_j^-)$$
(164)

and  $\sigma_i^+, \sigma_j^-$  are the Pauli spin matrices for creation and annihilation operators, n is the average number of connections to each neuron,  $w_{ij}$  is the synaptic transmission strength from the neuron j to neuron i,  $\alpha$  is the uniform decay rate and  $\psi$  is the generally nonlinear activation rate function. Although it is claimed by Penrose in his books [23], [24], neurons may not be quantized as a quantum superposition for both firing and not firing. However, for a hypothesized artificial quantum neural network, quantum superposition for the neuron states can be assumed. Therefore, it is natural to think about applying Lindblad equation as an analogous version to the results by Cowan.

Practically, the recently launched European Union Flagship of the Human Brain Project is hosted at EPFL in Switzerland which contains a subproject in Computational Neuroscience and Neurorobotics. It will provide mathematically oriented development for classical neuroscience. In addition, the 2045 Initiative pioneered by a Russian Billionaire Dmitry Itskov focuses on a final hologram-like avatar which is a robotic copy of a human body with a mind uploading technique.

This vista will strictly require us to reveal the functionality and structures in the human brain where modern mathematical tools are essential. Recently, there is a controversy model for consciousness introduced by Hameroff and Penrose [25], [26], [27], so-called Orch OR model. They believe that consciousness is generated from quantum microtubules. It may provide many open problems to the structures and dynamics of quantum microtubules which can be described by Cellular Automata.

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