

QUANTUM DECOHERENCE AND QUANTUM STATE DIFFUSION
FORMALISM

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ABSTRACT

QUANTUM DECOHERENCE AND QUANTUM STATE DIFFUSION FORMALISM

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Foundational problems of quantum theory, regarding the appearance of classicality and the measurement problem are stated and their link to studies of open quantum systems is discussed. This study's main aim is to analyze the main approaches that are employed in the context of open quantum systems. The general form of Markovian master equations are derived by a constructive approach. The Quantum State Diffusion (QSD) formalism is stressed upon as an alternative method to the master equations. Using the Caldeira-Leggett model in the context of QSD, stationary solutions of a charged particle exposed to a uniform magnetic field are found. The important points are summarized and the results are discussed.

Keywords: Open Quantum Systems, Decohorence, Quantum State Diffusion.

ÖZ

KUVANTUM UYUM KAYBI VE KUVANTUM DURUM DİFÜZYONU FORMALİZMİ

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Kuantum teorisindeki, klasik davranışın ortaya çıkması ve ölçüm problemini ilgilendiren temel problemleri açıklanmış, bunların açık kuantum sistemleri alanındaki çalışmalarla ilişkisi tartışılmıştır. Bu çalışmanın ana amacı açık kuantum sistemlerinde kullanılan genel yaklaşımları incelemektir. Markov özelliğine sahip temel denklemler yaklaşımsal olarak türetilmiştir. Kuantum Durum Difüzyonu(KDD) formalizmi temel denklem yaklaşımına alternatif bir metod olarak tanıtılıp üzerinde durulmuştur. Caldeira-Leggett modelini KDD formalizmi içerisinde kullanarak, düzgün manyetik alana tabi olan yüklü bir parçacığın kararlı çözümleri bulunmuştur. Önemli noktalar özetlenmiş ve sonuçlar tartışılmıştır.

Anahtar Kelimeler: Açık Kuantum Sistemleri, Uyum Kaybı, Kuantum Durum Difüzyonu Formalizmi

To Mom

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TABLE OF CONTENTS

ABSTRACT	iv
ÖZ	v
DEDICATION	vi
ACKNOWLEDGMENTS	vii
TABLE OF CONTENTS	viii
CHAPTER	
1 INTRODUCTION	1
1.1 Density Matrix	3
1.2 Entanglement	5
1.3 Decoherence	6
1.3.1 Correlation Dynamics	7
1.3.2 Diagonalization	8
2 REDUCED DYNAMICS AND MASTER EQUATIONS	10
2.1 The Reduced Dynamics	10
2.1.1 Generalized Master Equation	12
2.1.2 Markovian Master Equation	13
2.2 Important Aspects	24
2.2.1 Evolution of Diagonal Terms	24
2.2.2 Thermal Equilibrium and Markov Approximation	25
2.3 Quantum Brownian Motion	27
3 STOCHASTIC DYNAMICS	36
3.1 Wiener Process	36
3.2 Quantum State Diffusion	38
4 APPLICATION TO A MODEL	43
5 CONCLUSION	53
REFERENCES	56

CHAPTER 1

INTRODUCTION

The foundational problems of quantum mechanics like *measurement problem* and *emergence of classicality* have motivated physicists in order to establish the theory of open quantum systems. The research in open quantum systems has progressed over few past decades both at fundamental and phenomenological level. As the experimental techniques have been improved, open system dynamics became more important from the practical point of view. The understanding of decoherence and dissipation has become vital for the realization of quantum computers and for the progress of quantum computation. In this study main approaches to open systems are analyzed. In the first chapter, foundational issues are discussed along with preliminary subjects like density matrix, decoherence etc. In chapter 2, approaches to open systems are analyzed and derivations of master equations are given based on the physical assumptions. In the third chapter, the stochastic dynamics is introduced as a alternative approach to master equations. The ito calculus is dwelled upon and the *Quantum State Diffusion* (QSD) picture is introduced. In the following chapter, QSD is applied to a system consisting of a charged particle exposed to uniform magnetic field. In the LAST chapter, brief summary of important points is given and the results are discussed. In order to make a clear presentation of the subject, we begin with the foundational issues.

When we make a measurement on a system we find it to be in one of its *determinate* states in which the measured observable has a definite value. There is a fundamental assumption here; we may only observe the system in a determinate state in accordance with our experience. Why is that? What is the machinery that exactly turns the superposition of states into a single determinate state? This is the place where the problem arises. This problem in measurement theory is called as the *problem of*

definite outcomes[1].

One may easily see that there is a gap which must be filled quantitatively that will explain the physical state of affairs when a measurement takes place. von Neumann realized this gap and tried to solve the problem by proposing a postulate. This postulate simply states that the state vector representing the system reduces to one of its orthogonal bases after a measurement has occurred. This is called collapse of wavefunction or reduction of the state vector and it is non-unitary. According to one of the postulates of quantum mechanics, the state function describing a closed system evolves according to time dependent Schrödinger equation. The evolution of the state function is unitary and it is deterministic so that states evolve in a way that the norm and hence the total probability is conserved. However, von Neumann's postulate asserts that the system by the action of measurement evolves into one of its eigenstates in an indeterministic way and renormalizes itself when the measurement takes place. Considering this, there seems to be an inconsistency emerging when the collapse mechanism is introduced to the theory. On one side, we have continuous and deterministic time evolution of the states and on the other side, there emerges a discontinuity and indeterminacy brought by the collapse postulate which does not say much about what is going on during the measurement.

Associated with the measurement problem, there is the difficulty of so called the *classicality problem*. We perceive objects as having well defined position and momentum. The question then arises: Why we observe these properties as definite for these objects although they are made up of elementary particles which are treated as quantum mechanical? Put it another way how does a classical world emerge from the world of quantum? During the 1930s, it is commonly believed that, there should exist a borderline between the classical and quantum world. Classification of the objects as quantum and classical is important for determining the claimed borderline between the classical physics and quantum physics. The classicality is usually attributed to the macroscopic objects hence one may claim that having macroscopic properties is the fundamental criterion for classicality. However, recent advances show that the macroscopic entities can behave quantum mechanically. The Weber Bar, a gravity wave detector, is treated as a quantum harmonic oscillator and it weighs a ton.[2] Therefore, having macroscopic properties is not a solid criterion for a physical entity to be classical. Making the proper distinction between classical and Quantum mechanical

is important in order to fully understand the classicality problem.

To confront these setbacks, several approaches have been proposed. Some approaches deal with the interpretation of quantum mechanics while some other views bring modifications to the theory introducing stochastic versions of the Schrödinger equation. The Schrödinger equation is valid for closed systems and this is too idealistic for the real state of affairs since a system is immersed into an environment and is in interaction with it. This fact is central to the context of open quantum systems. In this scheme, Decoherence formalism is employed and master equations for the density matrices are analyzed. The effects of the environment on a specified system are investigated by using such master equations.

1.1 Density Matrix

Density matrices are widely used in approaches to open quantum systems. This need may be based upon several facts. The system under observation can be an ensemble of electrons. It can be a statistical mixture such that half of the electrons are prepared in the state A and the other half in the state B , which may be orthonormal to state A . One does not have to have an ensemble of electrons to use the density matrix; it may be utilized when there is a single electron. Assuming that one tosses a fair coin to prepare the electron's state such that if it is heads, the electron is prepared in state A ; otherwise it is prepared in state B . Therefore, the electron will be in state A or B with $\frac{1}{2}$ probability. In this case one may be tempted to write the electron's state as

$$|\psi\rangle = \frac{1}{\sqrt{2}}|A\rangle + \frac{1}{\sqrt{2}}|B\rangle. \quad (1.1)$$

However, state above implies that the electron is in a superposition of the states A and B , which has completely different properties. The electron is neither in state A nor in B , when one makes a measurement, the electron will be in state A or B with $\frac{1}{2}$ probabilities for each. These probabilities are related to the nature of the system. However, in the mentioned, scenario, the electron was prepared to be either in state A or B with a probability $\frac{1}{2}$ for each. The probability notion here is quite different. The state of the electron was prepared by flipping a coin; the classical probability defines the state of electron. Therefore, the state vector formalism is not suitable for such a preparation scheme. The preparation method is important because it can change the physical results. This fact can be made clearer by an example. Assuming that the

electron's spin state is given as

$$|\psi\rangle = \frac{1}{\sqrt{2}}|x_\uparrow\rangle + \frac{1}{\sqrt{2}}|x_\downarrow\rangle. \quad (1.2)$$

Then the probability of finding electron's spin up in the z direction is 1. If one prepares the state to be either in spin up or spin down in x direction with a $\frac{1}{2}$ probability for each, then probability of finding electron's spin up in the z direction becomes $\frac{1}{2}$. A convenient way of mathematical representation of the latter state is through the density matrix formalism,

$$\rho = \frac{1}{2}|x_\uparrow\rangle\langle x_\uparrow| + \frac{1}{2}|x_\downarrow\rangle\langle x_\downarrow|. \quad (1.3)$$

For a more generic state, density matrix can be written as

$$\rho = \sum_{i=1} w_i |\phi_i\rangle\langle\phi_i|, \quad (1.4)$$

which is equivalent to

$$\rho = \sum_{i,n,m} w_i c_{ni} c_{mi}^* |n\rangle\langle m|, \quad |\phi_i\rangle = \sum_n c_{ni} |n\rangle$$

in some orthonormal basis. Here, w_i is the weight corresponding to the classical probabilities; the probability of the state being prepared in $|\phi_i\rangle$. From the definition of generic mixed state it is obvious that density matrices are Hermitian matrices. The expectation of an observable is given as

$$\begin{aligned} \langle A \rangle &= \sum_i w_i \langle A \rangle_i \\ &= \sum_i w_i \langle \phi_i | A | \phi_i \rangle \\ &= \sum_{i,n} w_i \langle \phi_i | n \rangle \langle n | A | \phi_i \rangle \\ &= \text{Tr}(\rho A). \end{aligned} \quad (1.5)$$

Normalization condition is given as

$$\text{Tr} \rho = 1, \quad (1.6)$$

with the property,

$$\rho > 0$$

The inequality above implies density matrices are positive-definite matrices. In other words, beginning from upper-left corner, all square matrices contained in ρ and ρ itself

have positive determinants. If the determinants are non-negative, then ρ is a positive semi-definite matrix which is denoted as.

$$\rho \geq 0$$

Time evolution equation for the density matrices is called von-Neumann equation, which is obtained by the Schrödinger equation.

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[H, \rho]. \quad (1.7)$$

1.2 Entanglement

If the correlation between the system and environment is weak, the total state ket can be written as a tensor product

$$|\psi\rangle = \sum_{nm} c_n d_m |n_A\rangle |m_B\rangle, \quad (1.8)$$

which yields the density matrix as

$$\rho = \sum_{n,m,l,k} c_n c_l^* d_m d_k^* |n_A\rangle |m_B\rangle \langle l_A| \langle k_B|. \quad (1.9)$$

Reduced density matrix of A can be obtained by taking a partial trace over B .

$$\begin{aligned} \rho_A &= Tr_B \rho \\ &= \sum_{n,l} c_n c_l^* |n_A\rangle \langle l_A|, \end{aligned} \quad (1.10)$$

where partial trace over A , yields the environment's density matrix

$$\rho_B = \sum_{m,k} d_m d_k^* |m_B\rangle \langle k_B|. \quad (1.11)$$

It is evident that if the systems are not correlated strongly, than the total density matrix of the composite system can be written as a tensor product of ρ_A and ρ_B .

$$\rho = \rho_A \otimes \rho_B. \quad (1.12)$$

On the other hand, if the coupling between the environment and the system is strong, the correlation between the systems A and B leads to entangled state.

$$|\psi\rangle = \sum_n c_n |n_A\rangle |n_B\rangle, \quad (1.13)$$

where $|n_A\rangle$ and $|n_B\rangle$ are orthonormal bases for the system A and B respectively. The corresponding density matrix would be

$$\rho = \sum_{n,m} c_n c_m^* |n_A\rangle |n_B\rangle \langle m_A| \langle m_B|. \quad (1.14)$$

Partial trace yields the density matrices of the systems A and B .

$$\begin{aligned} \rho_A &= \sum_n |c_n|^2 |n_A\rangle \langle n_A| \\ \rho_B &= \sum_n |c_n|^2 |n_B\rangle \langle n_B| \end{aligned} \quad (1.15)$$

It is important to see that unlike the previous case, in the case of entanglement, the total density matrix can not be written as a tensor product of ρ_A and ρ_B

$$\rho \neq \rho_A \otimes \rho_B. \quad (1.16)$$

The crucial point to be made is: in the analysis of reduced system dynamics total density matrix is favored to be in tensor product form for the sake of simplicity. However, due to interactions between the system and environment one expects correlations in ρ . On the other hand, if the coupling is weak and environment is assumed to be a large one within a thermal equilibrium, than it is reasonable to assume that the state of the environment does not change much. Therefore total density matrix even though the interaction can be approximated as a tensor product, even though the two subsystems are interacting.

$$\rho \approx \rho_A \otimes \rho_B. \quad (1.17)$$

This approximation scheme will be very useful in order to investigate the reduced system dynamics.

1.3 Decoherence

The fundamental concept that makes quantum theory interesting is the superposition principle. A density matrix representing a single system in a pure state, a state which is a superposition of base states $|n\rangle$, can be written as:

$$\rho = \sum_{n,m} c_n c_m^* |n\rangle \langle m|. \quad (1.18)$$

When one performs a measurement on the system to , it is left in one of its eigenstates with the corresponding probability. If the experimenter does not look at the outcome, he would represent the final density matrix as

$$\rho = \sum_n |c_n|^2 |n\rangle\langle n|. \quad (1.19)$$

If he looks at the outcome than his density matrix will be a pure one. In both cases, the off-diagonal terms are gone. It is natural to assume that the effect of measurement is to diagonalize the density matrix. The relevant question is: What is the mechanism for diagonalization?

1.3.1 Correlation Dynamics

The measurement process is accomplished by the establishment of correlations between the system and the measurement device. For a general representation, one may assume the system is in one of its eigenstates. The formation of correlations is achieved through the interaction Hamiltonian. For the sake of simplicity, the following interaction Hamiltonian can be given:

$$H_{AB} = \sum_n |n\rangle\langle n| \otimes A_n. \quad (1.20)$$

The projection operators and A_n acts on their respective Hilbert spaces. If the initial state of the AB system is $|n\rangle|x_0\rangle$, the time evolution gives the state at time t as

$$\begin{aligned} e^{-iH_{int}t} |n\rangle|x_0\rangle &= |n\rangle e^{-iA_n t} |x_0\rangle \\ &= |n\rangle |x(t)_n\rangle. \end{aligned} \quad (1.21)$$

where $|x(t)_n\rangle$ is the state of the system B at time t , which is entangled to state of the system A . If A is in a superposition state at the initial moment, It follows from the linearity of the evolution equation that

$$\begin{aligned} e^{-iH_{int}t} \sum_n c_n |n\rangle|x_0\rangle &= \sum_n c_n |n\rangle e^{-iA_n t} |x_0\rangle \\ &= \sum_n c_n |n\rangle |x(t)_n\rangle, \end{aligned} \quad (1.22)$$

In other words an entangled state is obtained at time t . It is important to realize that measurement is not completed yet since the state did not collapse to a base yet. This is why some authors use the terminology *premeasurement phase* for this stage, where the collapse postulate had not yet entered the picture[3].

1.3.2 Diagonalization

The total density matrix of the system A and measurement apparatus B can be written as

$$\rho_{AB} = \sum_{n,m} c_n c_m^* |n\rangle \langle x(t)_n | \langle m | \langle x(t)_m |. \quad (1.23)$$

Tracing over the degrees of freedom of environment, the reduced density matrix for the system A can be obtained.

$$\rho_A = \sum_{n,m} c_n c_m^* |n\rangle \langle m | \langle x(t)_m | x(t)_n \rangle. \quad (1.24)$$

Diagonal terms are left unchanged since $\langle x(t)_n | x(t)_n \rangle = 1$ but in general, the off-diagonal terms decrease. The off-diagonal terms correspond to interference terms. As the system evolves, the decay of interference terms would give the diagonal form of the density matrix which would designate possible outcomes of measurement and the probabilities. To be simple and concrete, one may consider the Stern-Gerlach experiment, where the electron's spin is observed as either up or down. Therefore its density matrix must be diagonal in its basis. According to the argument, this result must be triggered by the orthogonality property of the states of the apparatus, which corresponds to distinguishability of the different positions where the electron hits on the detection screen of the apparatus.

It is a fact that the objects are immersed into an environment in which, the interactions with the photons, air molecules, dust particles and even with the neutrinos are frequent. To gain a more general insight of this approach, the effect of environment, which is central to Decoherence program, must be taken into account. The correlation of the AB system with the environment can be represented by a similar treatment. The subsystem density matrix can be given as

$$\rho_A = \sum_{n,m} c_n c_m^* |n\rangle \langle m | \langle x(t)_m | x(t)_n \rangle \langle e(t)_m | e(t)_n \rangle, \quad (1.25)$$

where $|e(t)_n\rangle$ are the states of the environment that correlate to system A . In the general sense, the factor which is multiplied with the states of the system is called *correlation function* which depends on the nature of interaction and the properties of the environment. Decoherence program, in general, analyzes the evolution of the off-diagonal elements of the density matrix belonging to subsystem A by using an appropriate interaction Hamiltonian. It is employed in several models such as spin

interaction, in which the environment is considered as a spin bath. It has been shown that the subsystem density matrix attains approximately a diagonal form.[4]

It is important to point out that the given interaction Hamiltonian was specific. The operator that act on the system A was chosen as a projection so that the system's state is left undisturbed during the measurement. A more formal treatment can be given by a generic interaction Hamiltonian which is of the form

$$H_{AB} = \sum_i \alpha_i \beta_i, \quad (1.26)$$

where α_i and β_i are the operators in the Hilbert space of the system A and apparatus B respectively. It is important to point out that the interaction Hamiltonian must be Hermitian, while α_i and β_i do not have to. The formal treatment of evolution of the density matrix with a generic interaction Hamiltonian will be given in the next chapter.

It is important to stress that Decoherence program, deals with the density matrix and tests it for a given interaction whether it reaches the desired diagonal form through the use of master equations. The statement that decoherence solves the measurement problem is questionable since the state vectors do not come into play in this picture. However, decoherence gives useful insights into the problem of classicality and this is the main motive for studying its aspects. Analysis of several systems reveals important quantities like decoherence time and decoherence length which are

CHAPTER 2

REDUCED DYNAMICS AND MASTER EQUATIONS

For a closed system, the evolution is determined by Schrödinger's equation once the initial conditions are known. However for bipartite or multipartite systems, computing the whole system's wavefunction in most cases is impossible. This is because one has to specify also the states of the environment which may have large degrees of freedom however, true concern in most circumstances is the subsystem's evolution. Therefore, procedures to get the reduced system dynamics were produced. Nakajima and Zwanzig[5] have introduced a projection method to split the external degrees of freedom from the open system which will be covered briefly in the next section. Another approach was presented by Feynman and Vernon which is based on *influence functional* for the representation of the effects induced by external environment[6].

2.1 The Reduced Dynamics

Projection operator technique is widely used in statistical physics for operations on the density matrices. Density matrices are defined on the space $\mathcal{D}(\mathcal{H})$. $\mathcal{D}(\mathcal{H})$ is the subset of the space of operators $\mathcal{T}(\mathcal{H})$, in which all the operators have finite and unique trace[7]. In this context, projection operator acts on $\mathcal{T}(\mathcal{H})$ and defined as a mapping that takes density matrix to an another density matrix. \mathcal{H} is the tensor product of the Hilbert spaces of system A and B

$$P : \rho \in \mathcal{D}(\mathcal{H}) \rightarrow P(\rho) \in \mathcal{D}(\mathcal{H}). \quad (2.1)$$

Projection operators have the following properties [7].

1. $P^2 = P$
2. $P(c\rho + d\rho') = cP\rho + dP\rho'$

$$3. \rho \geq 0 \Rightarrow P\rho \geq 0$$

$$4. \text{Tr}\{P\rho\} = 1.$$

The last two properties are not essential; they ensure that P conserves positivity and the trace. Hence, if ρ is a density matrix $P\rho$ is also. The operator $I - P$ is also a projection operator satisfying the first two properties above. The I is the identity operator of the state space. $I - P$ together with P satisfies

$$(I - P) + P = I, \quad (2.2)$$

$$(I - P)P = P(I - P) = 0. \quad (2.3)$$

The first relation indicates that operators P and $I - P$ divide $\mathcal{T}(\mathcal{H})$ into two subspaces. The second relation implies that these subspaces are linearly independent. Therefore, $\mathcal{T}(\mathcal{H})$ can be written as a direct sum of these subspaces. It follows that

$$(I - P)\rho + P\rho = \rho. \quad (2.4)$$

To analyze the subsystem dynamics, one must get the information regarding the system A from the generic state ρ . For this purpose, the projection operators are employed as a map taking ρ to its relevant part.

$$P : \rho \in \mathcal{D}(\mathcal{H}) \rightarrow \rho_{rel} \in \mathcal{D}(\mathcal{H}) \quad (2.5)$$

For Zwanzig type of projection, it gives

$$P(\rho) = (\text{Tr}_B \rho) \otimes \rho_B. \quad (2.6)$$

The tensor product is taken with the reference state $\rho_B \in \mathcal{D}(\mathcal{H}_B)$ so that $P(\rho)$ will be an element of $\mathcal{D}(\mathcal{H})$ which is consistent with P 's definition. The density matrix $P\rho$ is called the *relevant* part of the density matrix ρ , which contains statistical and quantum mechanical information regarding the system. The matrix $(I - P)\rho$ is the *irrelevant* part of the density matrix which does not enter into the calculation of expectation values [8]. According to von-Neumann equation

$$\frac{d\rho}{dt} = -\frac{i}{\hbar}[H, \rho(t)] = L\rho, \quad (2.7)$$

where H is the respective Hamiltonian of the system and environment plus the interaction Hamiltonian,

$$H = H_A \otimes I_E + H_E \otimes I_A + H_{AB}. \quad (2.8)$$

Equation (2.7) has a formal solution:

$$e^{Lt}\rho(0) = \rho(t), \quad (2.9)$$

where L is the generator of time evolution. For the relevant part, the Liouville equation reads

$$e^{\lambda t}\rho_{rel}(0) = \rho_{rel}(t), \quad (2.10)$$

where λ is the generator. To find the generator we first take the time derivative

$$\begin{aligned} \lambda e^{\lambda t}\rho_{rel}(0) &= \lambda\rho_{rel}(t) \\ &= \frac{d\rho_{rel}}{dt}. \end{aligned} \quad (2.11)$$

Using (2.10) and the definition of ρ_{rel} ,

$$\begin{aligned} \lambda P\rho(t) &= P\frac{d\rho}{dt} \\ &= PL\rho(t), \end{aligned} \quad (2.12)$$

thus, the generator must satisfy

$$\lambda\rho_{rel}(t) = PL\rho(t). \quad (2.13)$$

Likewise for the irrelevant part, the generator gives the relation

$$\lambda'(I - P)\rho(t) = (I - P)L\rho(t), \quad (2.14)$$

implying,

$$\lambda'\rho_{irrel}(t) = (I - P)L\rho(t). \quad (2.15)$$

2.1.1 Generalized Master Equation

If the density matrix is divided into relevant and irrelevant parts the conditions (2.13) and (2.15) can be used to obtain a set of coupled first order differential equations [7],

$$\begin{aligned} \frac{d(P\rho)}{dt} &= PLP\rho + PL(I - P)\rho, \\ \frac{d((I - P)\rho)}{dt} &= (I - P)LP\rho + (I - P)L(I - P)\rho. \end{aligned} \quad (2.16)$$

From these coupled equations one may get a generalized master equation for the subsystem's density matrix.

$$\frac{d\rho_A}{dt} = -\frac{i}{\hbar}[H', \rho_A(t)] + \int_0^t K(t-\tau)\rho_A(\tau)d\tau + R(t)\rho(0). \quad (2.17)$$

The operator in the integral and the third term in the sum are respectively:

$$\begin{aligned} K(t-\tau)\rho_A(\tau) &= Tr_E\{PL e^{(I-P)L(I-P)(t-\tau)}(I-P)LP\rho_A(\tau) \otimes \rho_B(\tau)\}, \\ R(t)\rho(0) &= Tr_B\{L(I-P)e^{(I-P)L(I-P)t}\rho_{irre}(0)\}, \end{aligned} \quad (2.18)$$

where the system Hamiltonian is given by

$$H' = H_A + Tr_B\{H_{AB}\rho_B\}. \quad (2.19)$$

This is an exact evolution equation for a system interacting with an environment for the choice of the projection operator given in (2.6). The integral in (2.17) indicates that the state of the system at time t depends on its state at time $t - \tau$, before t . This means that an excitation given to the environment by the system, returns back to system and affects its evolution. The whole effect of the prior states of the system on its present state is simply represented as an integral. The operator K contains the correlation functions of the environment. The last term in (2.17) stands for the correlations in the initial state. If the initial state is chosen as

$$\rho(0) = \rho_S(0) \otimes \rho_E \quad (2.20)$$

Then by definition the last term is zero since the system and environment are not entangled initially. The factorizing ansatz for the initial state would not lead to a loss of generality and in most applications the initial state is assumed to be factorizable. This is acceptable on the grounds that in non-equilibrium case of the subsystem, density matrix is expected to evolve to a stationary state which does not depend much on the initial state of the environment.

2.1.2 Markovian Master Equation

In a generic approach to the problem, the environment is large, weakly coupled to the system and it is considered to be in thermal equilibrium. Therefore, it is generally assumed that environment's state is stationary. During the interaction between the system and the environment, a kick given to the environment by the system, may

return to system itself after an arbitrarily long time. This leads to fluctuations on the system depending on its prior states. The return time of fluctuations depends on the correlation functions of the operators that couple environment to system. If these correlation functions decay on a timescale so short that no appreciable change in the system is observed, then one may assert that system's state at time $t+dt$ is determined by its state at time t . In other words, system is considered to be Markovian[9]. This is a reasonable statement on the grounds that the effect of the fluctuations are not resolved. Another way of putting it is that $K(t - \tau)$ in (2.18) is sharply peaked around time t hence it is proportional to the Dirac delta function: $\sim \delta(t)$. Based on several approximations, a Markovian master equation can be obtained for the system starting from the factorizing ansatz. The initial system-environment density matrix can be chosen as

$$\rho_{AB}(0) = \rho_A(0) \otimes \rho_B(0). \quad (2.21)$$

The Schrödinger equation is given as

$$\frac{d\rho_{AB}(t)}{dt} = -\frac{i}{\hbar}[H, \rho_{AB}(t)]. \quad (2.22)$$

During the interaction one may assume that the state of the reservoir does not change much due to weak coupling. This is the first assumption to be made.[10]

$$\rho_{AB}(t) = \rho_A(t) \otimes \rho_B(0). \quad (2.23)$$

Therefore,

$$\dot{\rho}_{AB}(t) = \dot{\rho}_A(t) \otimes \rho_B(0).$$

Decomposing the total Hamiltonian of the system and taking trace over the system B (i.e, the environment) puts (2.22) into

$$\begin{aligned} \dot{\rho}_A(t) = & -\frac{i}{\hbar}[H_A, \rho_A(t)] \\ & -\frac{i}{\hbar} Tr_B\{[H_B, \rho_B(0)]\rho_A(t)\} - \frac{i}{\hbar} Tr_B\{[H_{AB}, \rho_A(t) \otimes \rho_B(0)]\}. \end{aligned} \quad (2.24)$$

The identity operators in the Hamiltonian are acted on the respective density operators, which are taken out of commutators. Using the assumption that $\rho_B(0)$ does not evolve and the fact that its trace is 1, above equation reduces to

$$\dot{\rho}_A(t) = -\frac{i}{\hbar}[H_A, \rho_A(t)] - \frac{i}{\hbar} Tr_B\{[H_{AB}, \rho_A(t) \otimes \rho_B(0)]\}. \quad (2.25)$$

For an open system, it's more convenient to work with the interaction picture as in perturbation theory. Following transformations are made to switch from the Schrödinger picture to the interaction picture

$$\begin{aligned}(\rho_A(t) \otimes \rho_B(0))_{int} &= e^{\frac{i}{\hbar}(H_A \otimes I_B + H_B \otimes I_A)t} (\rho_A(t) \otimes \rho_B(0))_{sch} e^{-\frac{i}{\hbar}(H_A \otimes I_B + H_B \otimes I_A)t}, \\ H_{AB}(t)_{int} &= e^{\frac{i}{\hbar}(H_A \otimes I_B + H_B \otimes I_A)t} (H_{AB})_{sch} e^{-\frac{i}{\hbar}(H_A \otimes I_B + H_B \otimes I_A)t}.\end{aligned}$$

Time derivative of first equality yields

$$\begin{aligned}\dot{\rho}_A(t) \rho_B(0)_{int} &= \tag{2.26} \\ \frac{i}{\hbar} e^{\frac{i}{\hbar}(H_A \otimes I_B + H_B \otimes I_A)t} [(H_A \otimes I_B + H_B \otimes I_A), \rho_A(t) \otimes \rho_B(0)]_{sch} e^{-\frac{i}{\hbar}(H_A \otimes I_B + H_B \otimes I_A)t} \\ + e^{\frac{i}{\hbar}(H_A \otimes I_B + H_B \otimes I_A)t} \dot{\rho}_A(t) \otimes \rho_B(0)_{sch} e^{-\frac{i}{\hbar}(H_A \otimes I_B + H_B \otimes I_A)t}.\end{aligned}$$

Substitution of (2.25) for $\dot{\rho}_A(t)$, reduces the above equation to

$$\begin{aligned}\dot{\rho}_A(t) \rho_B(0)_{int} &= \tag{2.27} \\ -\frac{i}{\hbar} e^{\frac{i}{\hbar}(H_A \otimes I_B + H_B \otimes I_A)t} [H_{AB}, \rho_A(t) \otimes \rho_B(0)]_{sch} e^{-\frac{i}{\hbar}(H_A \otimes I_B + H_B \otimes I_A)t}.\end{aligned}$$

Leaving the commutator alone and taking trace yields

$$\begin{aligned}e^{-\frac{i}{\hbar}H_A t} \dot{\rho}_A(t)_{int} e^{\frac{i}{\hbar}H_A t} &= \tag{2.28} \\ -\frac{i}{\hbar} Tr_B \{ [H_{AB}, \rho_A(t) \otimes \rho_B(0)]_{sch} \}.\end{aligned}$$

Inserting it into (2.25), yields

$$\dot{\rho}_A(t) = -\frac{i}{\hbar} [H_A, \rho_A(t)] + e^{-\frac{i}{\hbar}H_A t} \dot{\rho}_A(t)_{int} e^{\frac{i}{\hbar}H_A t}. \tag{2.29}$$

To get a master equation for the density matrix, the second term must be simplified. In (2.28), leaving $\dot{\rho}_A(t)_{int}$ on left-hand side alone and inserting identity between $\rho_A(t) \otimes \rho_B(0)_{sch}$, H_{AB} and tracing gives the evolution equation for the density matrix in the interaction picture.

$$\dot{\rho}_A(t)_{int} = -\frac{i}{\hbar} Tr_B \{ [H_{AB}(t)_{int}, \rho_A(t)_{int} \otimes \rho_B(0)] \}. \tag{2.30}$$

From now on, it will be assumed that all expressions are in interaction picture, hence we will drop *int* index. Integrating the above equation from 0 to t ,

$$\rho_A(t) = \rho_A(0) - \frac{i}{\hbar} \int_0^t Tr_B \{ [H_{AB}(t'), \rho_A(t') \otimes \rho_B(0)] \} dt'. \tag{2.31}$$

Inserting $\rho_A(t)$ in (2.30)

$$\begin{aligned} \dot{\rho}_A(t) = & -\frac{i}{\hbar} Tr_B\{[H_{AB}(t), \rho_A(0) \otimes \rho_B(0)]\} \\ & -\frac{1}{\hbar^2} \int_0^t Tr_B\{[H_{AB}(t), [H_{AB}(t'), \rho_A(t') \otimes \rho_B(0)]]\} dt' \end{aligned} \quad (2.32)$$

The first assumption to be made in here is: $Tr_B\{H_{AB}(t)\rho_B(0)\}=0$, meaning that the operators that couple the reservoir (environment) to the system have zero average in the state $\rho_B(0)$. This can always be done by absorbing some terms from the interaction term into the system Hamiltonian. As already stated, due to interaction Hamiltonian, the system can give excitations to the environment and these excitations can return back after a certain time. Therefore, as indicated in the integral in (2.32), the system's evolution may depend on its prior states if the environment keeps the memory of the excitation. Naturally, the important to question to ask is that for how long this information is kept by the environment? Quantitatively this is given by the correlation functions of the environment, which give the correlation of the reservoir operators coupling to system at different times. If these functions decay in a time before $\rho_A(t')$ evolves significantly then it can be asserted that prior states of $\rho_A(t)$ does not affect its future evolution. Hence, $\rho_A(t')$ can be replaced by $\rho_A(t)$. This is known as Markov assumption. It holds if

$$\tau_A \gg \tau_B,$$

where τ_A is the time for a appreciable change in ρ_A and τ_B is the time required for bath correlation function decay. Interaction Hamiltonian can be chosen as a product of operators acting on Hilbert spaces \mathcal{H}_A and \mathcal{H}_B . Depending on the degrees of the freedom of system and environment, a general interaction Hamiltonian can be written as a linear combination of the product of operators. In the interaction picture

$$H_{AB} = \sum_i \alpha(t)_i \beta(t)_i. \quad (2.33)$$

For reasons that shall be clear, it is useful to express the system operators α_i as a sum of operators that excite the system states by a definite energy $\hbar\omega$ as follows [10]:

$$\alpha_i = \sum_{\omega} \alpha(\omega)_i, \quad (2.34)$$

$$\alpha(\omega)_i = \sum_{n,n'} P_n \alpha_i P_{n'}, \quad E_{n'} - E_n = \hbar\omega, \quad (2.35)$$

where P_n corresponds to the projection operator for the eigenspace of the system with the energy eigenvalue E_n . It is defined as

$$P_n = |\psi_n\rangle\langle\psi_n|, \quad (2.36)$$

$$H_A P_n = E_n |\psi_n\rangle\langle\psi_n|,$$

where $|\psi_n\rangle$ is the eigenstate state of H_A with eigenvalue E_n . The definition (2.35) is useful since it enables us to write the following relations.

$$[H_A, \alpha(\omega)_i] = -\omega\alpha(\omega)_i, \quad (2.37)$$

$$[H_A, \alpha^\dagger(\omega)_i] = \omega\alpha^\dagger(\omega)_i,$$

$$[H_A, \alpha^\dagger(\omega)_i\alpha(\omega)_j] = 0.$$

These equations enables us to express the system operators in interaction picture in a convenient form which facilitate a simple interpretation of the master equation. The operational meaning of $\alpha(\omega)_i$ becomes more clear when the commutation relations are acted to an energy eigenket.

$$H_A \alpha^\dagger(\omega)_i |\psi_n\rangle - \alpha^\dagger(\omega)_i H_A |\psi_n\rangle = \hbar\omega |\psi_n\rangle, \quad (2.38)$$

$$H_A \alpha^\dagger(\omega)_i |\psi_n\rangle = (E_n + \hbar\omega) \alpha^\dagger(\omega)_i |\psi_n\rangle.$$

In other words, if the operator $\alpha^\dagger(\omega)_i$ shifts the energy of the state by $\hbar\omega$. The interaction picture operators are

$$\alpha(\omega, t)_i = e^{\frac{i}{\hbar}H_A t} \alpha(\omega)_i e^{-\frac{i}{\hbar}H_A t} \quad (2.39)$$

Using Baker-Campbell-Hausdorff formula and the commutation relations, we obtain

$$\alpha(\omega, t)_i = e^{-i\omega t} \alpha(\omega)_i. \quad (2.40)$$

Similarly;

$$\alpha^\dagger(\omega, t)_i = e^{i\omega t} \alpha^\dagger(\omega)_i. \quad (2.41)$$

Using (2.40) and (2.41) the total interaction Hamiltonian can be written in the following form

$$\begin{aligned} \sum_i \alpha(t)_i \beta(t)_i &= \sum_{i,\omega} e^{-i\omega t} \alpha(\omega)_i \beta(t)_i \\ &= \sum_{i,\omega} e^{i\omega t} \alpha^\dagger(\omega)_i \beta^\dagger(t)_i. \end{aligned} \quad (2.42)$$

Writing $\sum_{i,\omega} e^{i\omega t} \alpha^\dagger(\omega)_i \beta^\dagger(t)_i$ for $H_{AB}(t)$ and $\sum_{j,\omega'} e^{-i\omega' t'} \alpha(\omega')_j \beta(t')_j$ for $H_{AB}(t')$, inserting into (2.38) and taking trace gives

$$\begin{aligned}
& -\frac{1}{\hbar^2} \int_0^t Tr_B \{ [H_{AB}(t), [H_{AB}(t'), \rho_A(t) R_B(0)]] \} dt' = \\
& -\frac{1}{\hbar^2} \sum_{i,j,\omega,\omega'} \int_0^t e^{-i\omega' t'} e^{i\omega t} \alpha^\dagger(\omega)_i \alpha(\omega')_j \rho_A(t) \langle \beta_i^\dagger(t) \beta_j(t') \rangle dt' \\
& + \frac{1}{\hbar^2} \sum_{i,j,\omega,\omega'} \int_0^t e^{-i\omega' t'} e^{i\omega t} \alpha(\omega)_j \rho_A(t) \alpha^\dagger(\omega)_i \langle \beta_i^\dagger(t) \beta_j(t') \rangle dt' \\
& - \frac{1}{\hbar^2} \sum_{i,j,\omega,\omega'} \int_0^t e^{-i\omega' t'} e^{i\omega t} \rho_A(t) \alpha(\omega')_j \alpha^\dagger(\omega)_i \langle \beta_j(t') \beta_i^\dagger(t) \rangle dt' \\
& + \frac{1}{\hbar^2} \sum_{i,j,\omega,\omega'} \int_0^t e^{-i\omega' t'} e^{i\omega t} \alpha^\dagger(\omega)_i \rho_A(t) \alpha(\omega')_j \langle \beta_j(t') \beta_i^\dagger(t) \rangle dt'.
\end{aligned} \tag{2.43}$$

Interaction Hamiltonian is hermitian, thus switching the operators to their hermitian conjugates in the last summation does not alter the equation.

$$\begin{aligned}
& -\frac{1}{\hbar^2} \int_0^t Tr_B \{ [H_{AB}(t), [H_{AB}(t'), \rho_A(t) R_B(0)]] \} dt' = \\
& -\frac{1}{\hbar^2} \sum_{i,j,\omega,\omega'} \int_0^t e^{-i\omega' t'} e^{i\omega t} \alpha^\dagger(\omega)_i \alpha(\omega')_j \rho_A(t) \langle \beta_i^\dagger(t) \beta_j(t') \rangle dt' \\
& + \frac{1}{\hbar^2} \sum_{i,j,\omega,\omega'} \int_0^t e^{-i\omega' t'} e^{i\omega t} \alpha(\omega)_j \rho_A(t) \alpha^\dagger(\omega)_i \langle \beta_i^\dagger(t) \beta_j(t') \rangle dt' \\
& - \frac{1}{\hbar^2} \sum_{i,j,\omega,\omega'} \int_0^t e^{i\omega' t'} e^{-i\omega t} \rho_A(t) \alpha^\dagger(\omega')_j \alpha(\omega)_i \langle \beta_j^\dagger(t') \beta_i(t) \rangle dt' \\
& + \frac{1}{\hbar^2} \sum_{i,j,\omega,\omega'} \int_0^t e^{i\omega' t'} e^{-i\omega t} \alpha(\omega)_i \rho_A(t) \alpha^\dagger(\omega')_j \langle \beta_j^\dagger(t') \beta_i(t) \rangle dt'.
\end{aligned} \tag{2.44}$$

Substituting t' by $t - \tau$ and interchanging the new integration limits with a minus sign, the equation reduces to

$$\begin{aligned}
& -\frac{1}{\hbar^2} \int_0^t Tr_B \{ [H_{AB}(t), [H_{AB}(t'), \rho_A(t) R_B(0)]] \} dt' = \\
& -\frac{1}{\hbar^2} \sum_{i,j,\omega,\omega'} \gamma_{ij} e^{i(\omega-\omega')t} \{ \alpha^\dagger(\omega)_i \alpha(\omega')_j \rho_A(t) - \alpha(\omega')_j \rho_A(t) \alpha^\dagger(\omega)_i \} \\
& - \frac{1}{\hbar^2} \sum_{i,j,\omega,\omega'} \gamma_{ji}^* e^{-i(\omega-\omega')t} \{ \rho_A(t) \alpha^\dagger(\omega')_j \alpha(\omega)_i - \alpha(\omega)_i \rho_A(t) \alpha^\dagger(\omega')_j \},
\end{aligned} \tag{2.45}$$

where

$$\gamma_{ij}(\omega) = \int_0^t e^{-i\omega\tau} \langle \beta_i^\dagger(t) \beta_j(t-\tau) \rangle d\tau. \tag{2.46}$$

For a continuum of frequencies, the summation in (2.45) turns into integration over the frequency range. The upper integration limit in (2.46) can be replaced by ∞ . This

will not change the integral significantly since the oscillating terms in the integral will average it to zero. This approximation gets better if the τ is much larger τ_B , the required time for correlation functions to decay. Therefore one may define γ_{ij} as the Fourier transform of the correlation functions which would be useful during the analysis of the specified environment-system interaction.

During the analysis of a open system, comparison of physical time scales are important in that it allows for sound assumptions. As already mentioned, two dynamical timescales are τ_A and τ_B . The fact that $\tau_A \gg \tau_B$ makes the fluctuations due to system's prior states unresolvable thus enables a Markovian description. The use of the definition (2.34) becomes apparent when τ_A is considered. Quantitatively, say for a two level atom in interaction with the electromagnetic field, τ_A would be proportional to $\sim \hbar|E_2 - E_1|^{-1}$ Where E_1 and E_2 correspond to two energy levels of the system. In this sense, for generic case, τ_A would be proportional to $\sim |\omega - \omega'|^{-1}$. The sought master equation naturally defines the subsystem's evolution from a non-equilibrium towards an equilibrium condition. The third important physical timescale is τ_R , the time it takes a system to reach equilibrium. If $\tau_R \gg \tau_A$ holds and the relevant observation time of the system is comparable to the relaxation time than

$$|\omega - \omega'| \tau \gg 1. \quad (2.47)$$

This means that the exponential in (2.45) wildly oscillates and the oscillating terms $\omega \neq \omega'$ may be ignored since the major contribution would come from diagonal terms. This approximation can be stated as some version of Rotating Wave Approximation[10]. Therefore, equation (2.45) reduces to

$$\begin{aligned} -\frac{1}{\hbar^2} \int_0^t Tr_B \{ [H_{AB}(t), [H_{AB}(t'), \rho_A(t) R_B(0)]] \} dt' = & \quad (2.48) \\ -\frac{1}{\hbar^2} \sum_{i,j,\omega} \gamma_{ij}(\omega) \{ \alpha^\dagger(\omega)_i \alpha(\omega)_j \rho_A(t) - \alpha(\omega)_j \rho_A(t) \alpha^\dagger(\omega)_i \} \\ -\frac{1}{\hbar^2} \sum_{i,j,\omega} \gamma_{ji}^*(\omega) \{ \rho_A(t) \alpha^\dagger(\omega)_j \alpha(\omega)_i - \alpha(\omega)_i \rho_A(t) \alpha^\dagger(\omega)_j \}. \end{aligned}$$

Due to interaction, the Hamiltonian of the system changes. Correction to the system Hamiltonian becomes apparent if γ_{ij} can be decomposed into its real and imaginary parts;

$$\begin{aligned} \frac{1}{\hbar^2} \gamma_{ij}(\omega) &= \frac{1}{2} \lambda_{ij}(\omega) + \frac{i}{\hbar} \chi_{ij}(\omega), \\ \frac{1}{\hbar^2} \gamma_{ji}^*(\omega) &= \frac{1}{2} \lambda_{ji}(\omega) - \frac{i}{\hbar} \chi_{ji}(\omega). \end{aligned} \quad (2.49)$$

The coefficients are demanded to be real. Inserting above expressions into (2.48)

$$\begin{aligned}
-\frac{1}{\hbar^2} \int_0^t Tr_B \{ [H_{AB}(t), [H_{AB}(t'), \rho_A(t) R_B(0)]] \} dt' = & \quad (2.50) \\
& - \sum_{i,j,\omega} \frac{1}{2} \lambda_{ij}(\omega) \{ \alpha^\dagger(\omega)_i \alpha(\omega)_j \rho_A(t) - \alpha(\omega)_j \rho_A(t) \alpha^\dagger(\omega)_i \} \\
& - \sum_{i,j,\omega} \frac{1}{2} \lambda_{ji}(\omega) \{ \rho_A(t) \alpha^\dagger(\omega)_j \alpha(\omega)_i - \alpha(\omega)_i \rho_A(t) \alpha^\dagger(\omega)_j \} \\
& + \sum_{i,j,\omega} \frac{i}{\hbar} \chi_{ij}(\omega) \{ \alpha(\omega)_j \rho_A(t) \alpha^\dagger(\omega)_i - \alpha^\dagger(\omega)_i \alpha(\omega)_j, \rho_A(t) \} \\
& + \sum_{i,j,\omega} \frac{i}{\hbar} \chi_{ji}(\omega) \{ \rho_A(t) \alpha^\dagger(\omega)_j \alpha(\omega)_i - \alpha(\omega)_i \rho_A(t) \alpha^\dagger(\omega)_j \}.
\end{aligned}$$

Exchanging the indices i and j in the second and fourth terms above,

$$\begin{aligned}
\dot{\rho}_A(t)_{int} = & \sum_{i,j,\omega} \lambda_{ij}(\omega) \{ \alpha(\omega)_j \rho_A(t) \alpha^\dagger(\omega)_i - \frac{1}{2} \{ \alpha^\dagger(\omega)_i \alpha(\omega)_j, \rho_A(t) \} \} \quad (2.51) \\
& - i \sum_{i,j,\omega} \frac{i}{\hbar} \chi_{ij}(\omega) [\alpha^\dagger(\omega)_i \alpha(\omega)_j, \rho_A(t)].
\end{aligned}$$

Switching back to the Schrödinger picture,

$$\begin{aligned}
e^{-\frac{i}{\hbar} H_A t} \dot{\rho}_A(t)_{int} e^{\frac{i}{\hbar} H_A t} = & - \sum_{i,j,\omega} \frac{i}{\hbar} \chi_{ij}(\omega) e^{-\frac{i}{\hbar} H_A t} [\alpha^\dagger(\omega)_i \alpha(\omega)_j, \rho_A(t)] e^{\frac{i}{\hbar} H_A t} \quad (2.52) \\
& + \sum_{i,j,\omega} \lambda_{ij}(\omega) e^{-\frac{i}{\hbar} H_A t} \{ \alpha(\omega)_j \rho_A(t) \alpha^\dagger(\omega)_i \} e^{\frac{i}{\hbar} H_A t} \\
& - \sum_{i,j,\omega} \lambda_{ij}(\omega) \frac{1}{2} e^{-\frac{i}{\hbar} H_A t} \{ \alpha^\dagger(\omega)_i \alpha(\omega)_j, \rho_A(t) \} e^{\frac{i}{\hbar} H_A t}.
\end{aligned}$$

Since H_A commutes with $\alpha^\dagger(\omega)_i \alpha(\omega)_j$, it can be readily seen that in second and third terms the only change is that $\rho_A(t)$ becomes $\rho_A(t)_{sch}$. Using (2.40) and (2.41) and inserting identities between $\rho_A(t)$ and the operators, above equation yields

$$\begin{aligned}
e^{-\frac{i}{\hbar} H_A t} \dot{\rho}_A(t)_{int} e^{\frac{i}{\hbar} H_A t} = & - \sum_{i,j,\omega} \frac{i}{\hbar} \chi_{ij}(\omega) [\alpha^\dagger(\omega)_i \alpha(\omega)_j, \rho_A(t)_{sch}] \quad (2.53) \\
& + \sum_{i,j,\omega} \lambda_{ij}(\omega) \{ \alpha(\omega)_j \rho_A(t)_{sch} \alpha^\dagger(\omega)_i \\
& - \sum_{i,j,\omega} \lambda_{ij}(\omega) \frac{1}{2} \{ \alpha^\dagger(\omega)_i \alpha(\omega)_j, \rho_A(t)_{sch} \} \}.
\end{aligned}$$

Using equation (2.29), and the master equation in Schrödinger picture is obtained.

$$\begin{aligned}
\dot{\rho}_A(t) = & -\frac{i}{\hbar} [H_A + H_C, \rho_A(t)] \quad (2.54) \\
& \sum_{i,j,\omega} \lambda_{ij}(\omega) \{ \alpha(\omega)_j \rho_A(t) \alpha^\dagger(\omega)_i - \frac{1}{2} \{ \alpha^\dagger(\omega)_i \alpha(\omega)_j, \rho_A(t) \} \}.
\end{aligned}$$

Where H_C is the correction Hamiltonian

$$H_C = \sum_{i,j,\omega} \chi_{ij}(\omega) \alpha^\dagger(\omega)_i \alpha(\omega)_j. \quad (2.55)$$

The sum in equation (2.54) can be put into diagonal form if λ matrix is positive-definite[10]. According to relations in (2.49) λ_{ij} is given by

$$\begin{aligned} \lambda_{ij}(\omega) &= \frac{1}{\hbar^2} \gamma_{ij}(\omega) + \frac{1}{\hbar^2} \gamma_{ij}^* \\ &= \frac{1}{\hbar^2} \int_0^\infty e^{-i\omega\tau} \langle \beta_i^\dagger(t) \beta_j(t-\tau) \rangle d\tau + \frac{1}{\hbar^2} \int_0^\infty e^{i\omega\tau} \langle \beta_i^\dagger(t-\tau) \beta_j(t) \rangle d\tau. \end{aligned} \quad (2.56)$$

It is important to see that correlation functions depend on the difference between the time arguments of the operators β_i^\dagger and β_j . Since it is assumed that reservoir's state is stationary one may rewrite correlation functions as

$$\begin{aligned} \langle \beta_i^\dagger(t) \beta_j(t-\tau) \rangle &= Tr_B \{ \rho_B \beta_i^\dagger(t) \beta_j(t-\tau) \} \\ &= Tr_B \{ \rho_B e^{\frac{i}{\hbar} H_B(t-\tau)} \beta_i^\dagger(\tau) e^{-\frac{i}{\hbar} H_B(t-\tau)} e^{\frac{i}{\hbar} H_B(t-\tau)} \beta_j(0) e^{-\frac{i}{\hbar} H_B(t-\tau)} \} \\ &= Tr_B \{ \rho_B e^{-\frac{i}{\hbar} H_B(t-\tau)} e^{\frac{i}{\hbar} H_B(t-\tau)} \beta_i^\dagger(\tau) \beta_j(0) \} \\ &= Tr_B \{ \rho_B \beta_i^\dagger(\tau) \beta_j(0) \}. \end{aligned} \quad (2.57)$$

The third step is written by using the cyclic property of the trace. Afterwards, H_B and ρ_B were swapped since they commute. Using the equality above $\lambda_{ij}(\omega)$ can be rewritten as

$$\lambda_{ij}(\omega) = \frac{1}{\hbar^2} \int_0^\infty e^{-i\omega\tau} \langle \beta_i^\dagger(\tau) \beta_j(0) \rangle d\tau + \frac{1}{\hbar^2} \int_0^\infty e^{i\omega\tau} \langle \beta_i^\dagger(-\tau) \beta_j(0) \rangle d\tau. \quad (2.58)$$

Changing dummy τ to $-\tau$ in the second integration,

$$\begin{aligned} \lambda_{ij}(\omega) &= \frac{1}{\hbar^2} \int_0^\infty e^{-i\omega\tau} \langle \beta_i^\dagger(\tau) \beta_j(0) \rangle d\tau - \frac{1}{\hbar^2} \int_0^{-\infty} e^{-i\omega\tau} \langle \beta_i^\dagger(\tau) \beta_j(0) \rangle d\tau \\ &= \frac{1}{\hbar^2} \int_{-\infty}^\infty e^{-i\omega\tau} \langle \beta_i^\dagger(\tau) \beta_j(0) \rangle d\tau. \end{aligned} \quad (2.59)$$

As can be seen readily, the elements of the matrix λ can be written as a full fourier transform of the correlation functions. If the matrix β such that

$$\beta_{ij} = \langle \beta_i^\dagger(\tau) \beta_j(0) \rangle$$

is positive-definite, then by Bochner's theorem[11], it is ensured that its Fourier transform is also positive-definite. Thus, in that case, one can entitle the λ matrix as a

positive-definite matrix. Therefore, λ matrix can be diagonalized by writing in the form

$$\lambda = A^{-1}vA, \quad (2.60)$$

where v is a diagonal matrix and $\lambda_{ij}(\omega)$ is represented as

$$\lambda(\omega)_{ij} = \sum_m a^*(\omega)_{im} v_{mm} a(\omega)_{mj}. \quad (2.61)$$

Using the above equation sum in (2.54) becomes

$$\sum_{i,j,m,\omega} a^*(\omega)_{im} v_{mm} a(\omega)_{mj} \{ \alpha(\omega)_j \rho_A(t) \alpha^\dagger(\omega)_i - \frac{1}{2} \{ \alpha^\dagger(\omega)_i \alpha(\omega)_j, \rho_A(t) \} \}$$

Defining the operators,

$$\begin{aligned} L_m^\dagger &= \sum_{i,\omega} a^*(\omega)_{im} \alpha^\dagger(\omega)_i, \\ L_m &= \sum_{j,\omega} a(\omega)_{mj} \alpha(\omega)_j. \end{aligned} \quad (2.62)$$

Inserting the above relations to (2.54) one obtains the so called *Lindbladian*.

$$\begin{aligned} \dot{\rho}_A(t) &= -\frac{i}{\hbar} [H'_A, \rho_A(t)] \\ &\quad \sum_m v_m \{ L_m \rho_A(t) L_m^\dagger - \frac{1}{2} \{ L_m^\dagger L_m, \rho_A(t) \} \}. \end{aligned} \quad (2.63)$$

The first term in equation (2.63) gives the internal evolution of system. The first term in the summation represents the transitions that the system may go through under the effect of environment. These transitions involve energy exchange so that dissipation enters the picture. Therefore summation part of the Lindbladian is usually called dissipative part. The other terms indicate the possibility that no transitions may occur. L_m and L_m^\dagger are called *Lindblad operators*. Lindblad operators need not be Hermitian or unitary since the system operators α_i do not have to. It is important to point out that Lindbladian is invariant under the following transformations of the Hamiltonian H'_A and Lindblad operators.[7]:

$$\begin{aligned} H'_A &\rightarrow H'_A - \frac{i}{2} \sum_{m>0} c_m^* L_m - c_m L_m^\dagger + d, \\ L_m &\rightarrow L_m + c_m, \end{aligned}$$

where c_m and d are scalars. Hence the Hamiltonian is not a unique operator. The master equation is also invariant under the unitary transformations which can be seen

readily from (2.62)

$$L_m \rightarrow \sum_l u_{lm} L_l.$$

Up to this point, Markovian master equation is constructed, starting from von-Neumann equation for a closed system. To get the reduced dynamics physically plausible approximations were made. The way followed to obtain (2.63) can be entitled as *constructive* approach[12]. Another method is the *axiomatic* approach which is mainly based on operator algebra rather than physical arguments. The importance of axiomatic approach is that it establishes the firm mathematical aspects of open system dynamics. The main starting point for this procedure is

$$\frac{d\rho(t)}{dt} = \mathcal{L}\rho(t) \quad (2.64)$$

$\rho(t)$ stands for the probability distribution of the system. The formal solution to (2.64) can be given as

$$\rho(t) = e^{\mathcal{L}t}\rho(0) \quad (2.65)$$

Obviously the operator $\phi_t = e^{\mathcal{L}t}$ maps the initial probability distribution to another one where \mathcal{L} is the operator generating the time translation. Consequently, ϕ_t becomes an operator that takes a density matrix and maps to another density matrix. From the properties of the density matrix one may infer that ϕ_t must conserve the trace. In other words, it must conserve the total probability. Besides, ϕ_t must be positive; it should map the positive elements of a set to positive elements of a different set. In the context of subsystem dynamics however, a stronger condition is needed. Ensuring that if $\rho_{AB}(0)$ is the initial density matrix of the composite system then, $\phi_t \otimes I_B \rho_{AB}(0)$ is also a density matrix. This means that if the system B does not evolve, regardless of the correlations between A and B , total density matrix should evolve to a new one. A map satisfying this property is called *completely positive* map[9]. G. Lindblad has shown that such a map satisfies the semigroup properties and derived (2.63) using operator algebra and dynamical semigroup properties[13].

$$\phi_0 = I : \text{The identity element}$$

$$\phi_t \phi_{t'} = \phi_{t+t'} : \text{The semigroup property.}$$

Lindblad's work is very important on the grounds that he has laid the mathematical foundations for an axiomatic approach to open system dynamics. According to

Kraus Representation theorem, any map satisfying the mentioned properties can be represented as[9].

$$\phi_t(\rho_A(0)) = \sum_n V_n^\dagger(t) \rho_A(0) V_n(t),$$

where $V_n(t)$ and $V_n^\dagger(t)$ are called *Kraus operators*. Since the trace must be preserved, they satisfy

$$\sum_n V_n(t) V_n^\dagger(t) = I, \quad (2.66)$$

where I stands for the identity. $V_n(t)$ and $V_n^\dagger(t)$ can be represented in terms of other Kraus operators by a unitary transformation,

$$V_n = \sum_l u_{nl} W_l$$

Thus the operator sum representation of ϕ_t is not unique. This is related to the reason why the Hamiltonian and Lindblad operators of (2.63) are not unique.

2.2 Important Aspects

2.2.1 Evolution of Diagonal Terms

The evolution of diagonal terms reveals an important property of (2.63). Representing the system Hamiltonian H_A in the energy bases, it can be seen that the first term in (2.54) gives no contribution. First note that

$$\begin{aligned} -\frac{i}{\hbar} \langle \psi_k | [H_A + H_C, \rho_A(t)] | \psi_k \rangle &= -\frac{i}{\hbar} \langle \psi_k | (H_A \rho_A(t) - \rho_A(t) H_A) | \psi_k \rangle \quad (2.67) \\ &= -\frac{i}{\hbar} \sum_{i,j,\omega} \chi_{ij}(\omega) \langle \psi_k | \alpha^\dagger(\omega)_i \alpha(\omega)_j \rho_A(t) | \psi_k \rangle \\ &\quad + \frac{i}{\hbar} \sum_{i,j,\omega} \chi_{ij}(\omega) \langle \psi_k | \rho_A(t) \alpha^\dagger(\omega)_i \alpha(\omega)_j | \psi_k \rangle, \end{aligned}$$

where

$$H_A = \sum_n E_n |\psi_n\rangle \langle \psi_n|. \quad (2.68)$$

It is clear that the first term yields zero. Using (2.37) the other terms yield

$$\begin{aligned} &-\frac{i}{\hbar} \sum_{i,j,\omega} \chi_{ij}(\omega) \langle \psi_k | [\alpha^\dagger(\omega)_i \alpha(\omega)_j, \rho_A(t)] | \psi_k \rangle = \\ &-\frac{i}{\hbar} \sum_{m,m'} \sum_{i,j,\omega} \chi_{ij}(\omega) \{ \rho_A(t)_{m'k} \langle \psi_k | \alpha_i^\dagger | \psi_m \rangle \langle \psi_m | \alpha_j | \psi_{m'} \rangle \\ &+ \rho_A(t)_{kl} \langle \psi_l | \alpha_i^\dagger | \psi_m \rangle \langle \psi_m | \alpha_j | \psi_k \rangle \}, \end{aligned}$$

which vanishes for diagonal elements. The second term of (2.54) yields an interesting result.

$$\begin{aligned} \sum_{i,j,\omega} \lambda_{ij} \{ (\omega) \langle \psi_k | \alpha(\omega)_j \rho_A(t) \alpha^\dagger(\omega)_i | \psi_k \rangle - \frac{1}{2} \langle \psi_k | \{ \alpha^\dagger(\omega)_i \alpha(\omega)_j, \rho_A(t) \} | \psi_k \rangle \} = \quad (2.69) \\ \sum_{m,l} \sum_{i,j,\omega} \lambda_{ij}(\omega) \{ \langle \psi_k | \alpha_i^\dagger | \psi_l \rangle \rho_A(t)_{lm} \langle \psi_m | \alpha_j | \psi_k \rangle - \frac{1}{2} \rho_A(t)_{kl} \langle \psi_l | \alpha_i^\dagger | \psi_m \rangle \langle \psi_m | \alpha_j | \psi_k \rangle \\ - \frac{1}{2} \rho_A(t)_{kl} \langle \psi_k | \alpha_i^\dagger | \psi_m \rangle \langle \psi_m | \alpha_j | \psi_l \rangle \}. \end{aligned}$$

For the diagonal terms $\rho_A(t)_{kk}$ master equation yields

$$\begin{aligned} \dot{\rho}_A(t)_{kk} = \sum_m \sum_{i,j} \lambda_{ij} (E_m - E_k) \{ \langle \psi_k | \alpha_i^\dagger | \psi_m \rangle \langle \psi_m | \alpha_j | \psi_k \rangle \rho_A(t)_{mm} \quad (2.70) \\ - \rho_A(t)_{kk} \langle \psi_k | \alpha_i^\dagger | \psi_m \rangle \langle \psi_m | \alpha_j | \psi_k \rangle \}. \end{aligned}$$

Equation (2.70) is the analog of Pauli master equation.

$$\frac{dP(t)_k}{dt} = \sum_m a_{km} P_m(t) - a_{mk} P_k(t) \quad (2.71)$$

The term a_{km} can be interpreted as the rate of transition from state k to state n while a_{mk} corresponds to the rate of transition from n to state k . Thus, Pauli equation represents a balanced in and out probability flow for the bases of the system. This is the analog of Chapman-Kolmogorov equation and both of them are Markovian. It can be concluded that the diagonal terms of the density matrix decouple from Lindbladian and obey Pauli master equation. Positivity of $\lambda_{ij}(E_m - E_k)$ assures that a map defined in this context; $\phi_t : \rho_A(0) \rightarrow \rho_A(t)$ preserves positivity.

2.2.2 Thermal Equilibrium and Markov Approximation

If the system is in interaction with an environment which is in the thermal equilibrium state

$$\begin{aligned} \rho_B = \frac{e^{-H_B \sigma}}{\text{Tr}_B e^{-H_B \sigma}}, \quad (2.72) \\ \sigma = \frac{1}{k_B T}, \end{aligned}$$

where, k_B is the Boltzmann's constant and T is temperature of the environment. The correlation function of the environment becomes

$$\langle \beta_i^\dagger(\tau) \beta_j(0) \rangle = \frac{\text{Tr}_B \{ e^{\frac{i}{\hbar} H_B \tau} \beta_i^\dagger(0) e^{-\frac{i}{\hbar} H_B \tau} \beta_j(0) e^{-H_B \sigma} \}}{\text{Tr}_B e^{-H_B \sigma}} \quad (2.73)$$

$$\begin{aligned}
&= \frac{\text{Tr}_B \{ \beta_j(0) e^{-H_B \sigma} e^{\frac{i}{\hbar} H_B \tau} \beta_i^\dagger(0) e^{-\frac{i}{\hbar} H_B \tau} e^{H_B \sigma} e^{-H_B \sigma} \}}{\text{Tr}_B e^{-H_B \sigma}} \\
&= \langle \beta_j(0) \beta_i^\dagger(\tau + \frac{i\sigma}{\hbar}) \rangle.
\end{aligned}$$

Above relation is called Kubo-Martin-Schwinger (KMS) condition. Taking the Fourier transforms of both sides, changing τ to $-\tau$ on the left-hand side and letting $\tau \rightarrow \tau + i\sigma$ on the right-hand side one obtains

$$\lambda_{ij}(-\omega) = e^{-\omega\sigma} \lambda_{ji}(\omega). \quad (2.74)$$

The important consequence of KMS relation and the reservoir being a canonical ensemble is that one expects the system to reach a thermal equilibrium state

$$\rho_A = \frac{e^{-H_A \sigma}}{\text{Tr}_A e^{-H_A \sigma}}, \quad (2.75)$$

In the state of equilibrium ρ_A is expected to be a stationary solution of the master equation, then

$$\dot{\rho}_A = 0 \quad (2.76)$$

This can be readily verified. Inserting (2.72) into (2.54), the first terms immediately yield zero since H_A commutes with H_C and itself. Further using (2.37) and (2.72) one may write the following relations

$$\begin{aligned}
\rho_A \alpha(\omega)_j &= e^{\omega\sigma} \alpha(\omega)_j \rho_A, \\
\rho_A \alpha^\dagger(\omega)_i &= e^{-\omega\sigma} \alpha^\dagger(\omega)_i \rho_A.
\end{aligned} \quad (2.77)$$

Replacing ω by $-\omega$ in the first relation in (2.37) and comparing with the second commutation relation, one may infer

$$\alpha(-\omega)_i = \alpha^\dagger(\omega)_i. \quad (2.78)$$

To verify that (2.75) indeed satisfies (2.76), it must be shown that the dissipative term in (2.54) gives no contribution. Changing ω to $-\omega$ in the first sum and exchanging the indices i and j gives

$$\begin{aligned}
&\sum_{i,j,\omega} \lambda_{ij}(\omega) \{ \alpha(\omega)_j \rho_A(t) \alpha^\dagger(\omega)_i - \frac{1}{2} \{ \alpha^\dagger(\omega)_i \alpha(\omega)_j, \rho_A(t) \} \} = \\
&\sum_{i,j,\omega} \lambda_{ji}(-\omega) \alpha(-\omega)_i \frac{e^{-H_A \sigma}}{\text{Tr}_A e^{-H_A \sigma}} \alpha^\dagger(-\omega)_j \\
&- \sum_{i,j,\omega} \frac{1}{2} \lambda_{ij}(\omega) \alpha^\dagger(\omega)_i \alpha(\omega)_j \frac{e^{-H_A \sigma}}{\text{Tr}_A e^{-H_A \sigma}} + \frac{e^{-H_A \sigma}}{\text{Tr}_A e^{-H_A \sigma}} \alpha^\dagger(\omega)_i \alpha(\omega)_j.
\end{aligned} \quad (2.79)$$

Using KMS relation, (2.74) and the last commutation relation in (2.44),

$$\sum_{i,j,\omega} e^{-\omega\sigma} \lambda_{ij}(\omega) \alpha^\dagger(\omega)_i \frac{e^{-H_A\sigma}}{\text{Tr}_A e^{-H_A\sigma}} \alpha(\omega)_j - \lambda_{ij} \alpha^\dagger(\omega)_i \alpha(\omega)_j \frac{e^{-H_A\sigma}}{\text{Tr}_A e^{-H_A\sigma}}.$$

Further using (2.78),

$$\sum_{i,j,\omega} \lambda_{ij}(\omega) \alpha^\dagger(\omega)_i \alpha(\omega)_j \frac{e^{-H_A\sigma}}{\text{Tr}_A e^{-H_A\sigma}} - \lambda_{ij} \alpha^\dagger(\omega)_i \alpha(\omega)_j \frac{e^{-H_A\sigma}}{\text{Tr}_A e^{-H_A\sigma}},$$

which is simply zero. Thus, the choice (2.75) is the invariant solution of the master equation.

Up this point, constructive derivation of the Markovian master equation is given with important aspects emphasized upon. It is important to point out that the Markovian master equation does not have a general applicability due to the assumptions made. Thus, it can at most give a phenomenological description. The main restriction on its generality is mainly due to the limitations of the Markov assumption. One of the subtlety is replacing $\rho_A(t')$ by $\rho_A(t)$ in (2.32). From the mathematical point of view, this step can be justified if $\langle \beta_i^\dagger(t) \beta_j(t') \rangle$ is $\sim C\delta(t - t')$, where C is some constant of the reservoir. However, for some reservoirs there may not be a natural timescale for decay or the decay rates may not be sufficiently fast endangering the Markov property. The validity of Markov property is restored if the integrand in (2.46) acts effectively $\delta(\tau)$ due to averaging effect of the $e^{i\omega\tau}$. This averaging effect is observed for a timescale comparable to the relaxation time of the system which again implies $\tau_R \gg \tau_A$.

The issue of renormalization is important. For the cases where system's bare Hamiltonian H_A diverges, finite frequency cut-off is introduced. From the definition of interaction Hamiltonian, it is readily seen that the correction coming to bare Hamiltonian, H_C , is cut-off dependent. As the cut-off limit goes to infinity the correction Hamiltonian diverges. However, the infinities in the bare Hamiltonian and the correction Hamiltonian must cancel themselves for renormalization.[12].

2.3 Quantum Brownian Motion

In the previous section, the demanded hierarchy between the relevant timescales made it possible to perform the Rotating Wave Approximation and to strengthen the Markov property. However, the inequality $\tau_R \gg \tau_A$ does not need to hold, in order to give

a Markovian prescription. There is alternative realization if the relevant timescales satisfy only

$$\tau_A \gg \tau_B$$

$$\tau_R \gg \tau_B.$$

Thus, the Rotating Wave approximation can not be employed as in (2.48). However, due to first inequality the reduced dynamics is strictly Markovian. The quantum version of the reduced dynamics is given by the so called Calderia-Leggett model[14]. The master equation can be derived by starting from equation (2.32), by choosing the interaction Hamiltonian as in (2.33). Inserting, $\sum_i \alpha_i(t)\beta_i(t)$ for $H_{AB}(t)$ and $\sum_i \alpha_j^\dagger(t)\beta_j^\dagger(t)$ for $H_{AB}(t')$, (2.38) yields

$$\begin{aligned} & -\frac{1}{\hbar^2} \int_0^t Tr_B \{ [H_{AB}(t), [H_{AB}(t'), \rho_A(t)R_B(0)]] \} dt' = \\ & -\frac{1}{\hbar^2} \sum_{i,j} \int_0^t \{ \alpha_i(t)\alpha_j^\dagger(t')\rho_A(t)\langle \beta_i(t)\beta_j^\dagger(t') \rangle - \alpha_j^\dagger(t')\rho_A(t)\alpha_i(t)\langle \beta_i(t)\beta_j^\dagger(t') \rangle \} dt' \\ & -\frac{1}{\hbar^2} \sum_{i,j} \int_0^t \{ \rho_A(t)\alpha_j^\dagger(t')\alpha_i(t)\langle \beta_j^\dagger(t')\beta_i(t) \rangle - \alpha_i(t)\rho_A(t)\alpha_j^\dagger(t')\langle \beta_j^\dagger(t')\beta_i(t) \rangle \} dt'. \end{aligned} \quad (2.80)$$

For convenience, the integration variable t' can be replaced by $t - \tau$.

$$\begin{aligned} & -\frac{1}{\hbar^2} \int_0^t Tr_B \{ [H_{AB}(t), [H_{AB}(t'), \rho_A(t)R_B(0)]] \} dt' = \\ & -\frac{1}{\hbar^2} \sum_{i,j} \int_0^t \alpha_i(t)\alpha_j^\dagger(t-\tau)\rho_A(t)\langle \beta_i(0)\beta_j^\dagger(-\tau) \rangle d\tau \\ & +\frac{1}{\hbar^2} \sum_{i,j} \int_0^t \alpha_j^\dagger(t-\tau)\rho_A(t)\alpha_i(t)\langle \beta_i(0)\beta_j^\dagger(-\tau) \rangle d\tau \\ & -\frac{1}{\hbar^2} \sum_{i,j} \int_0^t \rho_A(t)\alpha_j^\dagger(t-\tau)\alpha_i(t)\langle \beta_j^\dagger(-\tau)\beta_i(0) \rangle d\tau \\ & +\frac{1}{\hbar^2} \sum_{i,j} \int_0^t \alpha_i(t)\rho_A(t)\alpha_j^\dagger(t-\tau)\langle \beta_j^\dagger(-\tau)\beta_i(0) \rangle d\tau, \end{aligned} \quad (2.81)$$

where (2.57) is used to rewrite the correlation functions. For the reasons that will be clear each term in the integrand are expanded as below

$$\lambda = \frac{1}{2}\lambda - \frac{i^2}{2}\lambda. \quad (2.82)$$

Together with the definitions

$$\eta_1(\tau) = i\langle [\beta_i(0), \beta_j^\dagger(-\tau)] \rangle, \quad (2.83)$$

$$\eta_2(\tau) = \langle \{ \beta_i(0), \beta_j^\dagger(-\tau) \} \rangle,$$

equation (2.81) takes the form

$$\begin{aligned}
-\frac{1}{\hbar^2} \int_0^t Tr_B\{[H_{AB}(t), [H_{AB}(t'), \rho_A(t)R_B(0)]]\}dt' = & \quad (2.84) \\
-\frac{1}{2\hbar^2} \sum_{i,j} \int_0^t \eta_2(\tau)[\alpha_i(t), [\alpha_j^\dagger(t-\tau), \rho_A(t)]]d\tau \\
+\frac{i}{2\hbar^2} \sum_{i,j} \int_0^t \eta_1(\tau)[\alpha_i(t), \{\alpha_j^\dagger(t-\tau), \rho_A(t)\}]d\tau,
\end{aligned}$$

where the terms are taken into $\eta_1(\tau)$ and $\eta_2(\tau)$ parentheses by adding and subtracting $c\langle\beta_j^\dagger(-\tau)\beta_i(0)\rangle$ for each term like $c\langle\beta_i(0)\beta_j^\dagger(-\tau)\rangle$, and vice versa.

The Brownian motion is the relevant physical process in this picture. The motion of a particle which is exposed random collisions due to environment, (a gas, for instance) is a typical example of the Brownian motion. The Markovian nature of the Brownian motion ensures that the collisions suffered by the particle are statistically independent. In principle, physical nature of the interaction between the system and the environment in the Brownian motion is a scattering process. Thus, interaction Hamiltonian must couple the environment to the position space of the system. In addition, there may be energy exchange during the collisions resulting in momentum transfer. Thus, particle's evolution may be viewed as going from one point to another in the phase space. For a reservoir composed of harmonic oscillators in one dimension, the interaction Hamiltonian can be given as

$$\begin{aligned}
H_{AB}(t) &= -x \sum_n \kappa_n x_n & (2.85) \\
&= -x \sum_n \kappa_n \sqrt{\frac{\hbar}{2m_n\omega_n}} (b_n + b_n^\dagger),
\end{aligned}$$

where κ_n is the coupling constant of the n th oscillator. The reservoir Hamiltonian is evidently

$$H_B = \sum_n \hbar\omega_n b_n^\dagger b_n. \quad (2.86)$$

Using the prescribed interaction Hamiltonian, (2.84) becomes

$$\begin{aligned}
-\frac{1}{\hbar^2} \int_0^t Tr_B\{[H_{AB}(t), [H_{AB}(t'), \rho_A(t)R_B(0)]]\}dt' = & \quad (2.87) \\
-\frac{1}{2\hbar^2} \int_0^t \eta_2(\tau)[x(t), [x(t-\tau), \rho_A(t)]]d\tau \\
+\frac{i}{2\hbar^2} \int_0^t \eta_1(\tau)[x(t), \{x(t-\tau), \rho_A(t)\}]d\tau.
\end{aligned}$$

This expression is in interaction picture, the Schrödinger picture can be restored immediately with the following transformations and by using (2.29)

$$\begin{aligned}\rho_A(t)_{int} &= e^{\frac{i}{\hbar}H_A t} \rho_A(t)_{sch} e^{-\frac{i}{\hbar}H_A t} \\ x(t-\tau)_{int} &= e^{\frac{i}{\hbar}H_A t} x(-\tau)_{int} e^{-\frac{i}{\hbar}H_A t} \\ x(t)_{int} &= e^{\frac{i}{\hbar}H_A t} x(0)_{int} e^{-\frac{i}{\hbar}H_A t},\end{aligned}\tag{2.88}$$

where $x(0)_{int}$ naturally corresponds to x in Schrödinger picture. The upper integration limit can be taken to infinity as previously done since the bath correlations η_1 and η_2 are demanded to decay faster than any relevant timescale hence, the value of the integral will not be changed appreciably. Final form of the master equation becomes

$$\begin{aligned}\dot{\rho}_A(t) &= -\frac{i}{\hbar}[H_A, \rho_A(t)] - \frac{1}{2\hbar^2} \int_0^\infty \eta_2(\tau)[x, [x(-\tau), \rho_A(t)]]d\tau \\ &+ \frac{i}{2\hbar^2} \int_0^\infty \eta_1(\tau)[x, \{x(-\tau), \rho_A(t)\}]d\tau.\end{aligned}\tag{2.89}$$

According to the definition of the interaction Hamiltonian, there is a single bath operator and it is Hermitian. In the interaction picture it can be defined as

$$\begin{aligned}\beta_1(-\tau) &= e^{-\frac{i}{\hbar} \sum_i \hbar\omega_i b_i^\dagger b_i \tau} \sum_n \kappa_n \sqrt{\frac{\hbar}{2m_n\omega_n}} b_n e^{\frac{i}{\hbar} \sum_j \hbar\omega_j b_j^\dagger b_j \tau} \\ &+ e^{-\frac{i}{\hbar} \sum_i \hbar\omega_i b_i^\dagger b_i \tau} \sum_n \kappa_n \sqrt{\frac{\hbar}{2m_n\omega_n}} b_n^\dagger e^{\frac{i}{\hbar} \sum_j \hbar\omega_j b_j^\dagger b_j \tau}.\end{aligned}\tag{2.90}$$

By employing the Baker-Campbell-Hausdorff formula and the commutation relations it yields

$$\beta_1(-\tau) = \sum_n \kappa_n \sqrt{\frac{\hbar}{2m_n\omega_n}} b_n e^{i\omega_n \tau} + \sum_n \kappa_n \sqrt{\frac{\hbar}{2m_n\omega_n}} b_n^\dagger e^{-i\omega_n \tau}.\tag{2.91}$$

The environment is supposed to be thermal equilibrium. Thus,

$$\rho_B = \frac{\sum_n e^{-\frac{E_n}{k_B T}} |\psi_n\rangle\langle\psi_n|}{Tr\{\sum_n e^{-\frac{E_n}{k_B T}} |\psi_n\rangle\langle\psi_n|\}}.\tag{2.92}$$

E_n corresponds total energy of the reservoir, it is a summation of all oscillators' energies in the n th mode of environment. The term in the denominator corresponds to normalization. The numerator can be rewritten as

$$\begin{aligned}\sum_n e^{-\frac{E_n}{k_B T}} |\psi_n\rangle\langle\psi_n| &= e^{-\frac{H_B}{k_B T}} \sum_n |\psi_n\rangle\langle\psi_n| \\ &= e^{-\frac{1}{k_B T} \sum_i \hbar\omega_i b_i^\dagger b_i} \\ &= \prod_i e^{-\frac{1}{k_B T} \hbar\omega_i b_i^\dagger b_i}.\end{aligned}\tag{2.93}$$

The trace gives the normalization constant in the denominator and it is given as $(1 - e^{-\frac{\hbar\omega_i}{k_B T}})$ [15]. Thus, ρ_B becomes

$$\rho_B = \prod_i e^{-\frac{1}{k_B T} \hbar \omega_i b_i^\dagger b_i} (1 - e^{-\frac{\hbar\omega_i}{k_B T}}). \quad (2.94)$$

Using (2.91), the bath correlation function, $\langle \beta_1(0) \beta_1^\dagger(-\tau) \rangle$, becomes

$$\begin{aligned} \langle \beta_1(0) \beta_1^\dagger(-\tau) \rangle = & \quad (2.95) \\ & \sum_{i,k} \kappa_i \kappa_k \sqrt{\frac{\hbar}{2m_i \omega_i}} \sqrt{\frac{\hbar}{2m_k \omega_k}} e^{-i\omega_k \tau} \langle b_i b_k^\dagger \rangle \\ & + \sum_{i,k} \kappa_i \kappa_k \sqrt{\frac{\hbar}{2m_i \omega_i}} \sqrt{\frac{\hbar}{2m_k \omega_k}} e^{i\omega_k \tau} \langle b_i b_k \rangle \\ & + \sum_{i,k} \kappa_i \kappa_k \sqrt{\frac{\hbar}{2m_i \omega_i}} \sqrt{\frac{\hbar}{2m_k \omega_k}} e^{-i\omega_k \tau} \langle b_i^\dagger b_k^\dagger \rangle \\ & + \sum_{i,k} \kappa_i \kappa_k \sqrt{\frac{\hbar}{2m_i \omega_i}} \sqrt{\frac{\hbar}{2m_k \omega_k}} e^{i\omega_k \tau} \langle b_i^\dagger b_k \rangle. \end{aligned}$$

Second and third summations obviously yield zero. Inner product of Fock states of the environment dictates that only terms with $i = k$ survive hence,

$$\sum_{ik} \langle b_i^\dagger b_k \rangle = \sum_{ik} \delta_{ik} Tr\{\rho_B b_i^\dagger b_k\} \quad (2.96)$$

$$\begin{aligned} \sum_{ik} \langle b_i b_k^\dagger \rangle &= \sum_k Tr\{\rho_B b_k b_k^\dagger\} \\ &= \sum_k Tr\{\rho_B b_k^\dagger b_k\} + 1, \end{aligned} \quad (2.97)$$

with these definitions, (2.95) becomes

$$\begin{aligned} \langle \beta_1(0) \beta_1^\dagger(-\tau) \rangle &= \sum_k \kappa_k^2 \frac{\hbar}{2m_k \omega_k} e^{-i\omega_k \tau} (Tr\{\rho_B b_k^\dagger b_k\} + 1) \\ &+ \sum_k \kappa_k^2 \frac{\hbar}{2m_k \omega_k} e^{i\omega_k \tau} Tr\{\rho_B b_k^\dagger b_k\}. \end{aligned} \quad (2.98)$$

$Tr\{\rho_B b_k^\dagger b_k\}$ is given as

$$Tr\{\rho_B b_k^\dagger b_k\} = \frac{e^{-\frac{\hbar\omega_k}{k_B T}}}{1 - e^{-\frac{\hbar\omega_k}{k_B T}}}. \quad (2.99)$$

Using (2.98) $\eta_2(\tau)$ corresponds to

$$\eta_2(\tau) = \sum_k \kappa_k^2 \frac{\hbar}{2m_k \omega_k} e^{-i\omega_k \tau} (Tr\{\rho_B b_k^\dagger b_k\} + 1) \quad (2.100)$$

$$\begin{aligned}
& + \sum_k \kappa_k^2 \frac{\hbar}{2m_k \omega_k} e^{i\omega_k \tau} \text{Tr}\{\rho_B b_k^\dagger b_k\} \\
& + \sum_k \kappa_k^2 \frac{\hbar}{2m_k \omega_k} e^{-i\omega_k \tau} \text{Tr}\{\rho_B b_k^\dagger b_k\} \\
& + \sum_k \kappa_k^2 \frac{\hbar}{2m_k \omega_k} e^{i\omega_k \tau} (\text{Tr}\{\rho_B b_k^\dagger b_k\} + 1).
\end{aligned}$$

Organizing the terms

$$\eta_2(\tau) = \sum_k \kappa_k^2 \frac{\hbar}{2m_k \omega_k} \cos(\omega_k \tau) (\text{Tr}\{\rho_B b_k^\dagger b_k\} + \frac{1}{2}), \quad (2.101)$$

further using (2.99)

$$\text{Tr}\{\rho_B b_k^\dagger b_k\} + \frac{1}{2} = \coth\left(\frac{\hbar \omega_k}{2k_B T}\right), \quad (2.102)$$

which yields for a continuum of frequencies,

$$\eta_2(\tau) = \int_0^\infty J(\omega) \cos(\omega \tau) \coth\left(\frac{\hbar \omega}{2k_B T}\right) d\omega, \quad (2.103)$$

where

$$J(\omega) = \sum_k \kappa_k^2 \frac{\hbar}{2m_k \omega_k} \delta(\omega - \omega_k). \quad (2.104)$$

$J(\omega)$ corresponds to density of harmonic oscillators between the interval ω and $\omega + d\omega$, weighted by κ_k^2 and $\eta_2(\tau)$ corresponds to *Noise Kernel*[10]. It accounts for the random collisions suffered by the particle that causes the loss of coherence. In the same manner $\eta_1(\tau)$ yields

$$\eta_1(\tau) = \int_0^\infty J(\omega) \sin(\omega \tau) d\omega. \quad (2.105)$$

Physically, $\eta_1(\tau)$ corresponds to *Dissipation Kernel* of the environment. Its contribution quantifies the energy exchange of the system to reach the equilibrium. Explicit evaluation of noise and dissipation kernels give the decay rates which determines quantitatively the condition for the Markov approximation. This physical condition in turn, should make (2.103) and (2.105) proportional to $\delta(\tau)$ in order to justify the replacement of $\rho_A(t - \tau)$ with $\rho_A(t)$. In (2.104), $J(\omega)$ is defined in such a way that the kernels can be represented as an integral over continuous frequency range. The continuity of reservoir frequencies is favorable, because rates at which correlations must decay must be fast enough. In the case of discrete distribution of frequencies, the

correlation functions can be quasi-periodic. In that case non-Markovian fluctuations might occur. The main aim in this context is to obtain the irreversible dynamics of the system. For this reason, $J(\omega)$ is modified. Using (2.103) and (2.105), the inspection of time integrals in (2.89) indicates that there is a contribution from low frequency range. For practical purposes, $J(\omega)$ can be taken to be linear continuous function of ω in the low frequency range of environment[10].

$$J(\omega) = \frac{2m\gamma}{\pi}\omega, \quad (2.106)$$

where γ is introduced as a frequency independent damping constant characterizing the timescale to reach equilibrium. If the high frequency range is considered, a cut-off frequency Ω must be introduced for renormalization. Above definition can be improved by employing Lorenz-Drude cut-off function as a factor[10]

$$J(\omega) = \frac{2m\gamma}{\pi}\omega\frac{\Omega^2}{\Omega^2 + \omega^2}, \quad (2.107)$$

so that when the cut-off is taken to infinity, $J(\omega)$ reduces to (2.106). Using the definition above, noise and dissipation kernels can be found for a generic frequency,

$$\begin{aligned} \eta_1(\tau) &= 2m\gamma\hbar\Omega^2 e^{-\Omega|\tau|} \text{sign}(\tau), \\ \eta_2(\tau) &= 4m\gamma k_B T \Omega^2 \sum_{n=-\infty}^{\infty} \frac{\Omega e^{-\Omega|\tau|} - |\nu_n| e^{-|\nu_n||\tau|}}{\Omega^2 - \nu_n^2}, \end{aligned} \quad (2.108)$$

where ν_n is known as *Matsubara frequency*[10] which equals to $\frac{2\pi n k_B T}{\hbar}$. It is readily seen from the definitions that the relevant timescales for the decay of correlation functions are Ω^{-1} and ν_1^{-1} . For the Markov approximation to hold, we should have

$$\max(\Omega^{-1}, \nu^{-1}) \ll \omega_0^{-1},$$

where ω_0 corresponds to characteristic timescale of the system. The inequality above implies

$$\omega_0 \ll \min(\Omega, \nu_1). \quad (2.109)$$

$x(\tau)$ in (2.89) is can be denoted as

$$\text{Also, } x(\tau) = e^{-i\frac{H_A}{\hbar}\tau} x e^{i\frac{H_A}{\hbar}\tau}. \quad (2.110)$$

Considering (2.89), before the system evolves appreciably the kernels are supposed to decay hence $x(\tau)$ can be approximated up to order τ , which yields

$$\begin{aligned} x(\tau) &\approx x - \frac{i}{\hbar}[H_A, x]\tau \\ &\approx x - \frac{p}{m}\tau, \end{aligned} \quad (2.111)$$

where H_A is

$$H_A = \frac{p^2}{2m} + V(x). \quad (2.112)$$

Inserting (2.111) into (2.89), kernel part becomes

$$\begin{aligned} & \frac{1}{2\hbar^2} \int_0^\infty \{i\eta_1(\tau)[x, \{x(-\tau), \rho_A(t)\}] - \eta_2(\tau)[x, [x(-\tau), \rho_A(t)]]\} d\tau = \quad (2.113) \\ & - \frac{i}{2\hbar^2 m} \int_0^\infty \eta_1(\tau) \tau [x, \{p, \rho_A(t)\}] d\tau + \frac{i}{2\hbar^2} \int_0^\infty \eta_1(\tau) [x, \{x, \rho_A(t)\}] d\tau \\ & - \frac{1}{2\hbar^2} \int_0^\infty \eta_2(\tau) [x, [x, \rho_A(t)]] d\tau + \frac{1}{2\hbar^2 m} \int_0^\infty \eta_2(\tau) \tau [x, [p, \rho_A(t)]] d\tau. \end{aligned}$$

The evaluation of first and third term shows that dissipative and noise contributions to the reduced dynamics are at the low frequency range. In other words, time integrals yield $\sim \delta(\omega)$. The second term stands for the renormalization of the potential in the system Hamiltonian hence it can be absorbed into unnormalized Hamiltonian. The last integral involves the whole frequency domain, hence the high frequency noise effects are present. Thus it is dependent on the cut off frequency. It is approximately given by[10]

$$\frac{1}{2\hbar^2 m} \int_0^\infty \eta_2(\tau) \tau [x, [p, \rho_A(t)]] d\tau \approx \frac{2\gamma k_B T}{\hbar^2 \Omega} [x, [p, \rho_A(t)]]. \quad (2.114)$$

Inspection shows that as the cut-off is taken to ∞ , this term becomes negligible. Thus with the first and third terms in (2.113) integrated, the final form of the master equation becomes

$$\dot{\rho}_A(t) = -\frac{i}{\hbar} [H'_A, \rho_A(t)] - \frac{i\gamma}{\hbar} [x, \{p, \rho_A(t)\}] - \frac{2m\gamma k_B T}{\hbar^2} [x, [x, \rho_A(t)]], \quad (2.115)$$

where H'_A is the normalized Hamiltonian. It is important to note that, this equation is Markovian in the high temperature limit. Inspection on (3.29) shows that as the cut-off limit is taken to infinity, $\eta_1(\tau)$ becomes sharply peaked around $\tau = 0$, hence acts like $\delta(\tau)$. The demand for high temperature becomes apparent when $\eta_2(\tau)$ is observed. Despite the cut-off, the exponential $e^{-|\nu_n||\tau|}$ may not decay fast enough hence, it might cause a non-Markovian behavior. For the high temperature limit, the exponential will peak around zero, hence $\eta_2(\tau)$ will effectively behave like $\delta(\tau)$.

The prominent property of (2.115) is that it does not preserve the positivity of the density matrix, hence the generator of the evolution is not an element of dynamical semigroup. The fact that it violates positivity condition is easily seen if the second

term is expanded as

$$\begin{aligned}
-\frac{i\gamma}{\hbar}[x, \{p, \rho_A(t)\}] &= -\frac{i\gamma}{\hbar}(x\rho_A(t)p - p\rho_A(t)x) \\
&+ \frac{i\gamma}{2\hbar}(xp\rho_A(t) - \rho_A(t)px) \\
&+ \frac{i\gamma}{2\hbar}(xp\rho_A(t) - \rho_A(t)px).
\end{aligned} \tag{2.116}$$

Organizing the terms after adding and subtracting $-\frac{i\gamma}{2\hbar}(\rho_A(t)xp - px\rho_A(t))$, we get

$$\begin{aligned}
-\frac{i\gamma}{\hbar}[x, \{p, \rho_A(t)\}] &= -\frac{i\gamma}{\hbar}(x\rho_A(t)p - \frac{1}{2}\{px, \rho_A(t)\}) \\
&+ \frac{i\gamma}{\hbar}(p\rho_A(t)x - \frac{1}{2}\{xp, \rho_A(t)\}) \\
&- \frac{i\gamma}{2\hbar}[\{x, p\}, \rho_A(t)].
\end{aligned} \tag{2.117}$$

Absorbing the last term on the right-hand side into system Hamiltonian, the remaining terms correspond to dissipator in (2.54) with two system operators,

$$\alpha_1 = x, \quad \alpha_2 = p, \tag{2.118}$$

where the λ matrix becomes

$$\lambda = \begin{pmatrix} \frac{4m\gamma k_B T}{\hbar^2} & -\frac{i\gamma}{\hbar} \\ \frac{i\gamma}{\hbar} & 0 \end{pmatrix} \tag{2.119}$$

Since $\det\lambda$ is negative, the matrix is not positive-definite. However, as long as the high temperature limit is considered a term proportional to $\frac{1}{T}$ can be added to (2.115) so that the matrix becomes positive-definite. Positive λ ensures that it can be diagonalized hence Caldeira-Leggett master equation can be cast into Lindblad form. The condition for the positivity in the presence of λ_{22} is given as

$$\frac{4m\gamma k_B T}{\hbar^2}\lambda_{22} \geq \frac{\gamma^2}{\hbar^2}. \tag{2.120}$$

Obviously, if λ_{22} is assigned, the dissipator will gain an additional term $-\frac{\lambda_{22}}{2}[p, [p, \rho_A(t)]]$ which is proportional to $\frac{1}{T}$. Explicit form of Lindblad operators can be found by using (2.61), after diagonalizing λ for a convenient choice of λ_{22} .

CHAPTER 3

STOCHASTIC DYNAMICS

3.1 Wiener Process

The master equation represents the deterministic evolution of the probabilities and it is functional for studying open quantum systems and decohering effects of the environment. The Fokker-Planck equation in statistical physics may be considered as the classical analog of the Lindbladian. When analyzing a single system open to interaction, one may utilize the Fokker-Planck equation or directly consider the equation of motion by introducing stochastic elements. The stochastic approach to dynamics has advantages over the deterministic approach in regards to interpretational and computational issues[12].

In general, in stochastic approach, many realizations of the same event are performed and evolution patterns in each realization are observed. Main motive is to investigate whether there is a specified tendency in the process in addition to useful statistical information about a physical observable. Take the random walk case for example. If performed many times, one can get information about the statistical nature of a physical observable such as the distance x from the origin. If the random walk performed 100 times the occurrence count of the same value of x , say x_i , in principle can be equal to or smaller than 100 and in fact this corresponds to weight w_i in (1.6) in a statistical ensemble. Investigation shows that x_i versus occurrence count forms a normal type distribution peaked at $x_i = 0$, the initial point. equals zero. The distribution gets more continuous if the realization number gets higher. Quantitatively this statistical property leads to the fact that the average value of x will be 0. There is a type of stochastic process of special interest in the study of open quantum systems which is called *Wiener process*. Wiener process is a type of stochastic process in which the Markovian assumption holds. An incremental change in a stochastic variable in

time dt , belonging to a Wiener process is given as

$$dx = a(x, t)dt + b(x, t)d\xi. \quad (3.1)$$

The First term indicates the drift term. It is the dominant term during the evolution. The second term is the stochastic term which is called as Wiener increment. In stochastic equations, it helps to model the random influences of the environment to the system. Its influence becomes apparent in a larger timescale than the timescale of intrinsic evolution of the system. Wiener increment is of the order \sqrt{dt} . It has the following important properties[12]:

1. The Wiener increment $d\xi$, forms a gaussian distribution with mean 0 and variance \sqrt{dt} .
2. The Wiener increments at different times are statistically independent. This is also known as the *independent increment* property.

The first property leads:

$$\begin{aligned} M(d\xi(t)) &= M(\xi(t + dt) - \xi(t)) = 0, \\ Md\xi(t)^2 &= dt, \end{aligned} \quad (3.2)$$

where M represents taking mean over the distribution of possible values. The second property can be represented mathematically as

$$Md\xi(t)d\xi(t') = 0, \quad (3.3)$$

when $t \neq t'$. If there are more than one sources that produce random effects and if these sources are statistically independent then the general normalization condition becomes

$$Md\xi_i(t)d\xi_j(t) = \delta_{ij}dt. \quad (3.4)$$

The well known Brownian motion in statistical mechanics is essentially a Wiener process. In the case of classical Brownian motion, particle's trajectory can be given as a combination of main drift term and a stochastic factor which indicates the random collisions suffered by the particle. The collisions are statistical in nature and they are not correlated as depicted in (3.3). In other words, particle's evolution is treated as Markovian.

When dealing with the stochastic dynamics, because of the Wiener increment of order \sqrt{dt} , the derivation and integration rules differ from ordinary calculus. Japanese mathematician Kiyoshi Ito has laid the foundations the mathematical formalism to facilitate the treatment of stochastic processes[16]. Basic notions of the Ito calculus are Ito integral and Ito's lemma. The latter one is widely used in stochastic treatments of the wave equation and it is a modification of the ordinary chain rule in calculus. Let χ be a stochastic variable with drift and Wiener terms

$$d\chi(x, t) = \alpha(x, t)dt + \beta(x, t)d\xi. \quad (3.5)$$

For a function of χ and t , $f(\chi, t)$, physically relevant question is: How much does $f(\chi, t)$ change after a time interval dt during its evolution ?

$$df = f(t + dt) - f(t).$$

Taylor expansion gives

$$f(t + dt) = f + \frac{\partial f}{\partial \chi}d\chi + \frac{\partial f}{\partial t}dt + \frac{1}{2}\frac{\partial^2 f}{\partial \chi^2}(d\chi)^2 + \frac{1}{2}\frac{\partial^2 f}{\partial t^2}(dt)^2 + \frac{\partial^2 f}{\partial t \partial \chi}dtd\chi + \dots \quad (3.6)$$

Using (3.3) and (3.5) and removing higher order terms than dt , above equation reduces to

$$f(t + dt) = f + \left[\frac{\partial f}{\partial \chi}\alpha(x, t) + \frac{\partial f}{\partial t} + \frac{1}{2}\frac{\partial^2 f}{\partial \chi^2}\beta^2(x, t) \right]dt + \frac{\partial f}{\partial \chi}\beta(x, t)d\xi. \quad (3.7)$$

$$df = \left[\frac{\partial f}{\partial \chi}\alpha(x, t) + \frac{\partial f}{\partial t} + \frac{1}{2}\frac{\partial^2 f}{\partial \chi^2}\beta^2(x, t) \right]dt + \frac{\partial f}{\partial \chi}\beta(x, t)d\xi. \quad (3.8)$$

Ito derivative differs from the ordinary derivative due to random term in $d\chi$. It is frequently employed in calculating differential change in the expectation value of an observable as well as the mean rate of change of the variances. These topics will be covered up in more detail in the next section.

3.2 Quantum State Diffusion

To make a quantum mechanical description of dynamics employing the stochastic approach, the stochastic wave equations have to be investigated. Thus, in these approaches wavefunction is considered as a stochastic variable. Quantum State Diffusion is one of these approaches that studies the stochastic dynamics of the state vector. The main tool of QSD is the Ito-Langevin equation. It can be derived from the Lindbladian (2.63), if the density matrix is defined as a mean over the pure states of the

system[17].

$$\begin{aligned}
|d\psi\rangle = & -\frac{i}{\hbar}H|\psi\rangle dt + \frac{1}{2} \sum_j (2\langle L_j^\dagger \rangle L_j - L_j^\dagger L_j - \langle L_j^\dagger \rangle \langle L_j \rangle) |\psi\rangle dt \\
& + \sum_j (L_j - \langle L_j \rangle) |\psi\rangle d\xi_j(t),
\end{aligned} \tag{3.9}$$

where ρ_A is defined as

$$\rho_A = M|\psi\rangle\langle\psi|. \tag{3.10}$$

The first term in (3.9) denotes the internal dynamics while the first summation stands for the dissipative effect that induces energy exchange in order to reach the equilibrium. It is also necessary for the normalization of $|\psi\rangle$ at all times. Last summation corresponds to the noise due to fluctuations which are characterized by the Wiener increments. In quantum mechanics, the Wiener increment has a complex part which is independent from its real part.

$$d\xi = d\xi_{Re} + id\xi_{Im}$$

$$M(d\xi_{Re}d\xi_{Im}) = 0$$

The normalization condition for complex Wiener increment becomes

$$M(d\xi_i(t)d\xi_j^*(t)) = \delta_{ij}dt \tag{3.11}$$

$$M(d\xi_i(t)d\xi_j(t)) = 0$$

In QSD picture, for a generic system, the exact solution of the Ito Langevin equation can be a formidable task but for a non-equilibrium process the system is expected to reach a stationary state independent of the initial state of the system. It is important to stress that QSD approach is a phenomenological picture since the Markov assumption must hold. The motivation for QSD lays on several facts[18]. Iterative solution of (3.9) can be given once the Lindblad operators are known. The wavefunction is specified by n complex numbers where n is the dimension of the Hilbert space of the system. As for the density matrix, this number obviously will be of the order of n^2 . Hence, the numerical solutions for most systems are easier to compute when compared with the Lindbladian solution. Numeric approach is based on the matrix multiplication. Once the initial input data is inserted, the state vector for time $t + dt$ can be obtained. In literature, this technique is frequently employed and stationary

states for several types of systems are found[19]. However, one must perform the iterative method many times in order to get a reasonable statistical information about stationary solutions.

QSD picture deals with the state vectors and can give more physical insight about decoherence. The initial pure state, $|\psi_t\rangle$ may evolve to possible stationary solutions by following a variety of paths. Thus one gets an ensemble of paths each of which has a corresponding weight. Hence, definition (3.10) implies that the density matrix is the ensemble average of the pure states over the paths. If the stationary solutions are well localized in the corresponding observable's space then the density matrix would be approximately in diagonal form. This seems as a more reasonable or intuitive explanation for the diagonal form of the density matrix than the master equations offer.

In QSD approach, it has been shown that for a Brownian particle with a localized potential, the stationary solutions are localized wavefunctions in the phase space[20]. The physical properties of the stationary solutions are important. The emergence of stationary states that are close to minimum uncertainty states might provide reasons for appearance of classicality through interaction with the environment. Given a generic system and environment, the rate at which the equilibrium is established indicates how rapid an initial state of the system approaches to an anticipated stationary state. The localization rate for a specified interaction may give useful ideas about the problem of measurement. Lindblad operators can be chosen to simulate a measurement like processes. The solutions of QSD might be promising if they achieve proper localization rates.

The time derivatives of expectation values of observables and their variances give valuable information about the localization. For a stochastic state vector, differential change in the observable as time goes from t to $t + dt$, differs from the ordinary Schrodinger one due to presence of complex Wiener increments. For an observable X , we have

$$\begin{aligned} d\langle X \rangle &= d\langle \psi | X | \psi \rangle \\ &= \langle d\psi | X | \psi \rangle + \langle \psi | X | d\psi \rangle + \langle d\psi | X | d\psi \rangle. \end{aligned} \tag{3.12}$$

The Wiener increment's contribution is included in the last term due to normalization condition (3.11). Expanding the above equation using (3.9) for $d\psi$ and keeping the

orders up to dt

$$\begin{aligned} \langle \psi | X | d\psi \rangle &= -\frac{i}{\hbar} \langle X H_A \rangle dt + \sum_m \langle X (L_m - \langle L_m \rangle) \rangle d\xi_m \\ &+ \frac{1}{2} \sum_m \left\langle (2X \langle L_m^\dagger \rangle L_m - X L_m^\dagger L_m - X \langle L_m^\dagger \rangle \langle L_m \rangle) \right\rangle dt. \end{aligned} \quad (3.13)$$

Using normalization condition, $\langle d\psi | X | d\psi \rangle$ yields

$$\begin{aligned} \langle d\psi | X | d\psi \rangle &= \sum_{m,l} \left\langle (L_l^\dagger - \langle L_l^\dagger \rangle) X (L_m - \langle L_m \rangle) \delta_{lm} \right\rangle dt \\ &= \sum_m \left\langle (L_m^\dagger - \langle L_m^\dagger \rangle) X (L_m - \langle L_m \rangle) \right\rangle dt. \end{aligned} \quad (3.14)$$

Taking the Hermitian conjugate of (3.13) and summing all the terms yields

$$\begin{aligned} d\langle X \rangle &= \frac{i}{\hbar} \langle [H_A, X] \rangle - \frac{1}{2} \sum_m \langle L_m^\dagger [L_m, X] + [X, L_m^\dagger] L_m \rangle dt \\ &+ \sum_m \sigma(X, L_m) d\xi_m + \sigma(L_m^\dagger, X) d\xi_m^*, \end{aligned} \quad (3.15)$$

where σ denotes the correlation between two operators,

$$\begin{aligned} \sigma(X, L_m) &= \langle X L_m \rangle - \langle X \rangle \langle L_m \rangle, \\ \sigma(L_m^\dagger, X) &= \langle L_m^\dagger X \rangle - \langle L_m \rangle^* \langle X \rangle. \end{aligned} \quad (3.16)$$

The differential change in the variance of X is given as

$$\begin{aligned} d(\Delta X)^2 &= d(\langle X^2 \rangle - \langle X \rangle^2) \\ &= d\langle X^2 \rangle - 2\langle X \rangle d\langle X \rangle - (d\langle X \rangle)^2. \end{aligned} \quad (3.17)$$

The differential change in the expectation is a stochastic term which may have a drift and a diffusion term

$$d\langle X \rangle = a(t)dt + b(t)d\xi \quad (3.18)$$

Integration gives the expectation of the stochastic variable at a specified time.

$$\langle X(\tau) \rangle - \langle X(0) \rangle = \int_0^\tau a dt + \int_0^\tau b d\xi \quad (3.19)$$

The first term on the right-hand side is the usual Riemann integral, while the second one is known as *Ito integral*. It stands for the overall effect of the random influences due to environment. More specifically, Brownian motion can be considered. The particle's trajectory resembles a crooked non-differentiable path due to random collisions. Since a and b are dependent on ξ , these integrals contain the cumulative contribution of these collisions.

Ito's lemma and Ito integral are the main ingredients to analyze the system in QSD picture. In the next chapter, we wish to analyze a charged particle in the magnetic field which is in interaction with a bath of harmonic oscillators in thermal equilibrium. Therefore, the aim is to utilize QSD picture by using the Caldeira-Leggett model. For this reason Caldeira-Leggett master equation must be cast into Lindblad form so that the Ito-Langevin equation can be obtained with the corresponding Lindblad operators.

CHAPTER 4

APPLICATION TO A MODEL

In this section, the Caldeira-Leggett model will be considered for a specific physical system. The system is composed of a particle with a charge $+q$ and is restricted move in x-y plane. The particle is subjected to uniform magnetic field B in the z direction and is open to interaction with the external environment. The self Hamiltonian of the particle is taken as minimal coupling.

$$H_A = \sum_i \frac{\pi_i^2}{2m}, \quad (4.1)$$

where π stands for the kinetic momentum,

$$\pi_i = p_i - \frac{q}{c} A_i, \quad (4.2)$$

and kinetic momenta satisfy the commutation relation,

$$[\pi_x, \pi_y] = iB \frac{q\hbar}{c}. \quad (4.3)$$

Fixing the gauge as rotationally invariant, we have

$$\begin{aligned} A_x &= -\frac{By}{2}, \\ A_y &= \frac{Bx}{2}. \end{aligned} \quad (4.4)$$

It is useful to introduce creation and annihilation operators so that the system can be treated as a harmonic oscillator.

$$\begin{aligned} a &= \sqrt{\frac{c}{2q\hbar B}} (\pi_x + i\pi_y) \\ a^\dagger &= \sqrt{\frac{c}{2q\hbar B}} (\pi_x - i\pi_y) \\ [a, a^\dagger] &= 1 \end{aligned} \quad (4.5)$$

The energy levels of the particle gets quantized due to boundary conditions imposed by the magnetic field. Definition in (4.5) yields the Hamiltonian of the system as

$$H_A = \hbar\omega \left(a^\dagger a + \frac{1}{2} \right), \quad (4.6)$$

where ω corresponds to cyclotron frequency $\frac{qB}{mc}$. Acting the annihilation operator on the ground states yields evidently zero, hence from the obtained differential equation, position space representation of the wavefunction can be found.

$$\begin{aligned} \langle x, y | a | 0 \rangle &= \sqrt{\frac{c}{2q\hbar B}} \langle x, y | (-i\hbar(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}) - \frac{qB}{2c}(-y + ix)) | 0 \rangle \quad (4.7) \\ &= -i\sqrt{\frac{\hbar c}{2qB}} \left((\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}) + \frac{qB}{2\hbar c}(x + iy) \right) \psi(x, y) \\ &= 0. \end{aligned}$$

Solution for the ground states can be given up to a arbitrary function $f(x, y)$, which must be periodic and analytic,[21] as follows,

$$\psi(x, y) = f(x, y) e^{-\frac{qB(x^2+y^2)}{4\hbar c}}. \quad (4.8)$$

Analytic means that $f(x, y)$ is an analytic function of $x + iy$. The arbitrariness in the choice of $f(x, y)$ yields degeneracy in the ground state. For the choice

$$f(x, y) = (x + iy)^m, \quad (4.9)$$

where m is a non-negative integer, ground state becomes

$$\psi_m(x, y) = (x + iy)^m e^{-\frac{qB(x^2+y^2)}{4\hbar c}}. \quad (4.10)$$

Hence the ground state is infinitely degenerate. These degenerate states are called the lowest Landau level. The excited states can be found by acting the creation operator on the ground state. For example, for the first excited states.

$$\begin{aligned} a^\dagger \psi_m(x, y) &= -i\sqrt{\frac{\hbar c}{2qB}} \left(\frac{\partial}{\partial x} - i\frac{\partial}{\partial y} \right) - \frac{qB}{2c} \left((x - iy)(x + iy)^m e^{-\frac{qB(x^2+y^2)}{4\hbar c}} \right) \quad (4.11) \\ &= -i\sqrt{\frac{\hbar c}{2qB}} \left(m(x + iy)^m + \frac{qB}{mc}(x^2 + y^2) \right) (x + iy)^{m-1} e^{-\frac{qB(x^2+y^2)}{4\hbar c}}. \end{aligned}$$

Further acting of the creation operator gives the other excited states which all have the same degeneracy.

The purpose is to find the stationary states of this system under the presence of quantum noise by using Ito-Langevin equation in the context of Caldeira-Leggett

model. Therefore the starting point is to specify the Lindblad operators. In order to employ the QSD equation for this system, the Caldeira Leggett model must be converted into Lindblad form. The environment is taken to be isotropic harmonics oscillators in two dimension. The environment Hamiltonian is given as

$$H_B = \sum_n \frac{p_{nX}^2}{2m_n} + \frac{m_n \omega_n^2 X^2}{2} + \sum_n \frac{p_{nY}^2}{2m_n} + \frac{m_n \omega_n^2 Y^2}{2}. \quad (4.12)$$

where n denotes the oscillator number. The treatment starts by specifying the interaction Hamiltonian as

$$H_{AB} = \sum_i x_i X_i \quad (4.13)$$

where i runs from 1 to 2, representing the coordinates of the particle. X_i can be written in the form

$$X_i = \sum_n \kappa_{ni} \sqrt{\frac{\hbar}{2m_n \omega_n}} (b_{ni} + b_{ni}^\dagger), \quad (4.14)$$

where n stands for the oscillator number. Inserting the interaction Hamiltonian into (2.87)

$$\begin{aligned} \dot{\rho}_A(t) = & -\frac{i}{\hbar} [H_A, \rho_A(t)] - \sum_{ij} \frac{1}{2\hbar^2} \int_0^\infty \eta_2(\tau) [x_i, [x_j(-\tau), \rho_A(t)]] d\tau \\ & + \sum_{ij} \frac{i}{2\hbar^2} \int_0^\infty \eta_1(\tau) [x_i, \{x_j(-\tau), \rho_A(t)\}] d\tau, \end{aligned} \quad (4.15)$$

where $\eta_1(\tau)$ and $\eta_2(\tau)$ are now given by

$$\begin{aligned} \eta_1(\tau) &= i \langle [X_i, X_j(-\tau)] \rangle \\ \eta_2(\tau) &= \langle \{X_i, X_j(-\tau)\} \rangle. \end{aligned}$$

$X_j(-\tau)$ is

$$X_j(-\tau) = \sum_m \kappa_{mj} \sqrt{\frac{\hbar}{2m_m \omega_m}} b_{mj} e^{i\omega_m \tau} + \sum_m \kappa_{mj} \sqrt{\frac{\hbar}{2m_m \omega_m}} b_{mj}^\dagger e^{-i\omega_m \tau}.$$

The term must yield $\langle X_i(0) X_j(-\tau) \rangle$ as

$$\begin{aligned} \langle X_i(0) X_j(-\tau) \rangle = & \delta_{ij} \sum_n \kappa_n^2 \frac{\hbar}{2m_n \omega_n} e^{-i\omega_n \tau} (Tr\{\rho_B b_n^\dagger b_n\} + 1) \\ & + \delta_{ij} \sum_n \kappa_n^2 \frac{\hbar}{2m_n \omega_n} e^{i\omega_n \tau} Tr\{\rho_B b_n^\dagger b_n\}. \end{aligned} \quad (4.16)$$

Corresponding kernels are modified by δ_{ij} factor which gives a diagonal form.

$$\begin{aligned} \dot{\rho}_A(t) = & -\frac{i}{\hbar} [H_A, \rho_A(t)] - \frac{1}{2\hbar^2} \int_0^\infty \eta_2(\tau) [x_i, [x_i(-\tau), \rho_A(t)]] d\tau \\ & + \frac{i}{2\hbar^2} \int_0^\infty \eta_1(\tau) [x_i, \{x_i(-\tau), \rho_A(t)\}] d\tau. \end{aligned} \quad (4.17)$$

Considering the system Hamiltonian, the approximation made in (2.111) becomes

$$x(\tau)_i \approx x_i - \frac{\pi_i}{m}\tau. \quad (4.18)$$

The corresponding master equation becomes

$$\begin{aligned} \dot{\rho}_A(t) = & -\frac{i}{\hbar}[H_A + \frac{\gamma}{2}\{x_i, \pi_i\}, \rho_A(t)] - \frac{i\gamma}{\hbar}[x_i, \{\pi_i, \rho_A(t)\}] \\ & - \frac{2m\gamma k_B T}{\hbar^2}[x_i, [x_i, \rho_A(t)]]. \end{aligned} \quad (4.19)$$

To make the λ matrices positive, λ_{22} must be introduced. For the least disturbance of the master equation, choosing λ_{22} as minimum, the master equation becomes

$$\begin{aligned} \dot{\rho}_A(t) = & -\frac{i}{\hbar}[H_A + \frac{\gamma}{2}\{x_i, \pi_i\}, \rho_A(t)] - \frac{i\gamma}{\hbar}[x_i, \{\pi_i, \rho_A(t)\}] \\ & - \frac{2m\gamma k_B T}{\hbar^2}[x_i, [x_i, \rho_A(t)]] - \frac{\gamma}{8mk_B T}[\pi_i, [\pi_i, \rho_A(t)]]. \end{aligned} \quad (4.20)$$

where λ_i is

$$\lambda_i = \begin{pmatrix} \frac{4m\gamma k_B T}{\hbar^2} & -\frac{i\gamma}{\hbar} \\ \frac{i\gamma}{\hbar} & \frac{\gamma}{4mk_B T} \end{pmatrix} \quad (4.21)$$

Lindblad operators are chosen as below to satisfy the diagonal form (2.63).

$$L_i = \frac{\sqrt{4mk_B T\gamma}}{\hbar}x_i + i\sqrt{\frac{\gamma}{4mk_B T}}\pi_i \quad (4.22)$$

The dissipation constant γ can be absorbed into coefficients. Change in the expectation values of observables can be given using (3.15) and the Lindblad operators above,

$$\begin{aligned} d\langle x_i \rangle &= \frac{\langle \pi_i \rangle}{m} dt + \sigma(x_i, L_m)d\xi_m + \sigma(L_m^\dagger, x_i)d\xi_m^*, \\ d\langle p_i \rangle &= \epsilon_{ij} \frac{\langle \pi_j \rangle}{2} \omega dt - 2\hbar ab \langle \pi_i \rangle dt + \sigma(p_i, L_m)d\xi_m + \sigma(L_m^\dagger, p_i)d\xi_m^*, \\ d\langle \pi_i \rangle &= \epsilon_{ij} \langle \pi_j \rangle \omega dt - 2\hbar ab \langle \pi_i \rangle dt + \sigma(\pi_i, L_m)d\xi_m + \sigma(L_m^\dagger, \pi_i)d\xi_m^*. \end{aligned} \quad (4.23)$$

where the repeated indices are to be summed over. ϵ_{ij} is the anti-symmetric tensor.

The constants a and b stand for the shorthand notation

$$a = \frac{\sqrt{4m\gamma k_B T\gamma}}{\hbar}, \quad (4.24)$$

$$b = \sqrt{\frac{\gamma}{4mk_B T}}. \quad (4.25)$$

The mean time derivative of variances are essential for analyzing the arbitrary and stationary states. Using (3.17) and the properties of the Wiener increments, following

relations are found for a generic state.

$$M \frac{d(\Delta x_i)^2}{dt} = \frac{2R_i}{m} + \hbar^2 b^2 - \epsilon_{ij} \sigma(x_i, x_j) - 2\sigma(x_i, L_{im})\sigma(L_{im}, x_i) \quad (4.26)$$

$$M \frac{d(\Delta p_i)^2}{dt} = -4ab\hbar\sigma(p_i, p_i) - \epsilon_{ij}\sigma(p_i, p_j) + \hbar^2 a^2 + 2\hbar abm\omega\sigma(p_i, x_j) \\ + \frac{1}{4}\hbar^2 a^2 b^2 \omega^2 - 2\sigma(x_i, L_{im})\sigma(L_{im}, x_i)$$

$$M \frac{d(R_i)}{dt} = \frac{\sigma(p_i, p_i)}{m} - \epsilon_{ij} \frac{\omega}{2} (\sigma(x_i, p_j) + \sigma(x_j, p_i)) - \frac{1}{4} m \omega^2 \sigma^2(x_i, x_i) \\ - 2\hbar ab R_i + \epsilon_{ij} \sigma(x, y) - \sigma(x_i, L_m) \sigma(L_m, p_i) + \sigma(p_i, L_m) \sigma(L_m, x_i)$$

$$M \frac{d\sigma(p_i, x_j)}{dt} = \frac{\sigma(p_i, p_j)}{m} + \epsilon_{ij} \frac{\omega}{2} (R_i - R_j) - \frac{m\omega^2}{4} \sigma(x_i, x_j) \\ - 2ab\hbar\sigma(p_i, x_j) + \epsilon_{ij}\hbar abm\omega\sigma(p_j, p_j) - \frac{\epsilon_{ij}}{2}\hbar^2 b^2 m\omega^2 \\ - \sigma(p_i, L_m)\sigma(L_m, x_j) + \sigma(L_m, p_i)\sigma(x_j, L_m)$$

where R_i corresponds to symmetric correlation of x_i and p_i .

$$R_i = \frac{1}{2}\sigma(x_i, p_i) + \frac{1}{2}\sigma(p_i, x_i). \quad (4.27)$$

The other mean time derivatives yield

$$M \frac{d\sigma(x, y)}{dt} = \frac{\sigma(p_x, y)}{m} + \frac{\sigma(p_y, x)}{m} + \frac{\omega}{2} (\sigma^2(x, x) + \sigma^2(y, y)) \quad (4.28) \\ - (\sigma(x, L_m)\sigma(L_m, y) + \sigma(L_m, x)\sigma(y, L_m)),$$

$$M \frac{d\sigma(p_x, p_y)}{dt} = \frac{\omega}{m} (\sigma(p_x, p_x) - \sigma(p_y, p_y)) - \frac{m\omega^2}{4} (\sigma(y, p_x) + \sigma(x, p_y)) \\ - 4\hbar ab\sigma(p_x, p_y) + \frac{1}{2}\hbar mab\omega(R_x - R_y) - \sigma(p_x, L_m)\sigma(L_m, p_y) \\ + \sigma(L_m, p_x)\sigma(p_y, L_m).$$

In order to find the stationary solutions, an analytically solvable algebraic equation has to be investigated. A useful algebraic relation can be given by employing a conjecture. In (4.20), positivity condition was imposed by adding a small term in the high temperature limit so that the equation can be modified to Lindblad form. If the system's evolution is given by Lindbladian and the environment is in thermal equilibrium, then the system's density matrix is expected to attain an approximately diagonal form as in section (2.2.2). In QSD picture, each diagonal element of the

density matrix correspond to pure states. In the context of Brownian motion, these correspond to states that are well localized in the phase space. In [20], it was conjectured that if the system reaches to a stationary solution than the variance of the phase space variables should be constant. Therefore in a time interval dt , stationary solution can change by a phase in addition to differential changes in the expectation values of the phase space variables is If the change in the phase is omitted, we have,

$$\begin{aligned} \psi_{t+dt} = & \psi_t - d\langle x_i \rangle \frac{i}{\hbar} p_i \psi_t + d\langle p_i \rangle \frac{i}{\hbar} x_i \psi_t - \frac{1}{2\hbar^2} d\langle x_i \rangle d\langle x_j \rangle p_i p_j \psi_t \\ & - \frac{1}{2\hbar^2} d\langle p_i \rangle d\langle p_j \rangle x_i x_j \psi_t + \frac{1}{\hbar^2} d\langle x_i \rangle d\langle p_j \rangle p_i x_j \psi_t + \dots \end{aligned} \quad (4.29)$$

which yields

$$\psi_{t+dt} = \exp\left\{\frac{i}{\hbar} d\langle p_i \rangle x_i - \frac{i}{\hbar} d\langle x_i \rangle p_i\right\} \psi_t. \quad (4.30)$$

On the other hand, Langevin-Ito equation implies,

$$\begin{aligned} \psi_{t+dt} &= \psi_t + \alpha |\psi\rangle dt + \beta_j |\psi\rangle d\xi_j \\ &= \exp\{\alpha dt + \beta_j d\xi_j\} \psi_t. \end{aligned} \quad (4.31)$$

The last equality is valid on the grounds that higher order terms than dt do not contribute and the normalization condition (3.11) implies

$$d\xi_i d\xi_j = 0. \quad (4.32)$$

Terms α and β_j correspond to

$$\begin{aligned} \alpha &= -\frac{i}{\hbar} H + \frac{1}{2} (2\langle L_j^\dagger \rangle L_j - L_j^\dagger L_j - \langle L_j^\dagger \rangle \langle L_j \rangle), \\ \beta_j &= L_j - \langle L_j \rangle. \end{aligned} \quad (4.33)$$

The stationary solutions must then satisfy

$$\exp\{\alpha dt + \beta_j d\xi_j\} |\psi\rangle = \exp\left\{\frac{i}{\hbar} x_i d\langle p_i \rangle - \frac{i}{\hbar} p_i d\langle x_i \rangle + \frac{i}{\hbar} d\phi\right\} |\psi\rangle, \quad (4.34)$$

where ϕ is included as a phase term which can be defined as a stochastic factor.

$$\phi = \phi_0 + \phi_m d\xi_m + \phi_m^* d\xi_m^* \quad (4.35)$$

Exponential operator on the right-hand side can be taken to the left by utilizing the formula

$$e^A e^B = e^{A+B} e^{\frac{1}{2}[A,B]}, \quad (4.36)$$

where,

$$\begin{aligned} [A, [A, B]] &= [B, [B, A]] \\ &= 0 \end{aligned} \quad (4.37)$$

must hold. When applying (4.36) to (4.34) α commutations does not bother because it is higher order than dt . Together with β commutations

$$e^{\{\alpha dt + \beta_j d\xi_j - \frac{i}{\hbar} x_i d\langle p_i \rangle + \frac{i}{\hbar} p_i d\langle x_i \rangle - \frac{i}{\hbar} d\phi + \frac{i}{2\hbar} [p_i, \beta_j] d\xi_j d\langle x_i \rangle - \frac{i}{2\hbar} [x_i, \beta_j] d\xi_j d\langle p_i \rangle\}} |\psi\rangle = |\psi\rangle. \quad (4.38)$$

Expanding the exponential up to first order we get

$$(A dt + B_m d\xi_m + C_m d\xi_m^*) |\psi\rangle = 0, \quad (4.39)$$

which implies the set of equations

$$\begin{aligned} A|\psi\rangle &= 0, \\ B_m|\psi\rangle &= 0, \\ C_m|\psi\rangle &= 0, \end{aligned} \quad (4.40)$$

where the coefficients are given as

$$\begin{aligned} A &= -\frac{i}{\hbar} \phi_0 + \alpha + p_i \frac{\langle \pi_i \rangle}{\hbar m} + 2iabx_i \langle \pi_i \rangle - \frac{i}{2\hbar} \epsilon_{ij} x_i \langle \pi_j \rangle \omega \\ &\quad + \frac{i}{4} bm\omega \epsilon_{im} \sigma(L_m^\dagger, x_i) + \frac{a}{2} \sigma(L_m^\dagger, x_m) - \hbar b \sigma(L_m^\dagger, p_m), \\ B_m &= \frac{i}{\hbar} p_i \sigma(x_i, L_m) - x_i \sigma(p_i, L_m) - \phi_m + L_m - \langle L_m \rangle, \\ C_m &= \frac{i}{\hbar} p_i \sigma(L_m^\dagger, x_i) - x_i \sigma(L_m^\dagger, p_i) - \phi_m^*. \end{aligned} \quad (4.41)$$

One may argue that the terms $B_m C_m$ and $C_m B_m$ which appears in the second order expansion of (4.38) must be taken into account since they are order of dt . However from (4.40) it follows that they do not contribute. (4.40) yields the differential equations for the wavefunctions

$$\begin{aligned} \langle x, y | B_m | \psi \rangle &= \left(\frac{\partial}{\partial x_i} - \frac{i}{\hbar} \langle p_i \rangle \right) \sigma(x_i, L_m) \psi + \frac{1}{2} ibm\omega \epsilon_{nm} x_n \psi \\ &\quad - \frac{i}{\hbar} \sigma(p_i, L_m) (x_i - \langle x_i \rangle) \psi + ax_m \psi + \hbar b \frac{\partial \psi}{\partial x_m} \end{aligned} \quad (4.42)$$

$$\langle x, y | C_m | \psi \rangle = \left(\frac{\partial}{\partial x_i} - \frac{i}{\hbar} \langle p_i \rangle \right) \sigma(L_m^\dagger, x_i) \psi - \frac{i}{\hbar} \sigma(L_m^\dagger, p_i) (x_i - \langle x_i \rangle) \psi \quad (4.43)$$

Phase is chosen such that the equations (4.42) and (4.43) would suggest a general solution which has a form in the position space as follows

$$\psi = Ne^{a_i(x_i - \langle x_i \rangle)^2 + b_i x_i + c(x_i - \langle x_i \rangle)(x_j - \langle x_j \rangle)}, \quad (4.44)$$

where N is the normalization constant. The momentum expectations determine the constants b_i

$$\begin{aligned} \langle p_k \rangle &= -i\hbar|N|^2 \int e^{(a_i + a_i^*)(x_i - \langle x_i \rangle)^2 + (b_i + b_i^*)x_i + (c + c^*)(x_i - \langle x_i \rangle)(x_j - \langle x_j \rangle)} \\ &\times \{2a_k(x_k - \langle x_k \rangle) + b_k + c(\delta_{kj}(x_i - \langle x_i \rangle) + c\delta_{ki}(x_j - \langle x_j \rangle))\}. \end{aligned} \quad (4.45)$$

The factors $(x_m - \langle x_m \rangle)$ in the integrand vanishes, hence

$$b_k = \frac{i}{\hbar} \langle p_k \rangle. \quad (4.46)$$

The remaining constants can be found by employing equation (4.41). Inserting (4.44) into (4.41) gives an equation of the form

$$E_i x_i^2 \psi + F x_i x_j \psi + G_i x_i \psi + H \psi = 0. \quad (4.47)$$

For x_i can take all real values, all the coefficients must vanish. E_i and F are given as

$$\begin{aligned} E_i &= -\frac{i}{2\hbar m} (-4a_i^2 \hbar^2 - \hbar^2 c^2 + i \sum_j \epsilon_{ij} \hbar m \omega c + \frac{1}{4} m^2 \omega^2 + 4ia_i \hbar^2 abm) \\ &- \frac{1}{2} (a^2 - 4a_i^2 b^2 \hbar^2 - \hbar^2 b^2 c^2 + i \sum_j \epsilon_{ij} \hbar b^2 m \omega c + \frac{1}{4} \hbar^2 b^2 \omega^2) \\ F &= -\frac{i}{2\hbar m} (4\hbar^2 \sum_i a_i c - 2i\hbar m \sum_{ij} \epsilon_{ij} \omega a_i + -4i\hbar^2 abmc) \\ &- \frac{1}{2} (4\hbar^2 b^2 c \sum_i a_i + 2i\hbar m \omega b^2 \sum_{ij} \epsilon_{ji} a_i) \end{aligned} \quad (4.48)$$

Above equations yield two roots for the constants. For normalization, a_i must satisfy

$$Re(a_i) < 0,$$

which yields the solution as

$$\begin{aligned} a_i &= -\frac{m\omega}{\hbar} \frac{2\mu\nu + \sqrt{(\nu^2 - i)^2 + \mu^2(8\nu^2 - 4i)}}{4(\nu^2 - i)}, \\ c &= 0, \end{aligned} \quad (4.49)$$

where

$$\begin{aligned}\mu &= \sqrt{\frac{4k_B T \gamma}{\hbar \omega^2}}, \\ \nu &= \sqrt{\frac{\hbar \gamma}{4k_B T}}.\end{aligned}\tag{4.50}$$

For ν equals to zero, a_i can be decomposed into its real and imaginary parts

$$\begin{aligned}Re(a_i) &= -\frac{m\omega}{\hbar} \frac{\mu^2}{\sqrt{2\sqrt{16\mu^4 + 1} - 2}} \\ Im(a_i) &= -\frac{m\omega}{\hbar} \frac{\sqrt{1 + \sqrt{16\mu^4 + 1}}}{4\sqrt{2}}\end{aligned}\tag{4.51}$$

It is important to note that the solution depends on the choice of gauge. In the rotationally symmetric gauge, a_i for both x and y components turned out to be equal. The uncertainties are

$$\begin{aligned}\sigma(x_i, x_i) &= -\frac{1}{2(a_i + a_i^*)}, \\ \sigma(p_i, p_i) &= \frac{2\hbar^2 |a_i|^2}{a_i + a_i^*}, \\ R_i &= \frac{i\hbar(a_i - a_i^*)}{2(a_i + a_i^*)}.\end{aligned}\tag{4.52}$$

The uncertainty relation is

$$\sigma(x_i, x_i)\sigma(p_i, p_i) - R_i^2 \geq \frac{\hbar^2}{4}\tag{4.53}$$

The equality is satisfied for the stationary state. Moreover, right-hand side of equation (4.26) must vanish for these states. The remaining variances yield zero since the stationary solution is a general gaussian type wavefunction. The correlation of Lindblad operators in the stationary state become

$$\begin{aligned}\sigma(x_i, L_j) &= -\frac{a\delta_{ij}}{2(a_i + a_i^*)} - \frac{\delta_{ij}\hbar b a_i}{a_i + a_i^*} + \frac{m\omega\epsilon_{ji}}{4c(a_i + a_i^*)}, \\ \sigma(p_i, L_j) &= -\frac{i\hbar a\delta_{ij}}{a_i + a_i^*} + \frac{2ib\delta_{ij}\hbar^2 |a_i|^2}{a_i + a_i^*} - \frac{\hbar b^2 m\omega a_i \epsilon_{ji}}{a_i + a_i^*}.\end{aligned}\tag{4.54}$$

The stationary state can be characterized as the eigenvalues of the operators ζ_i such that

$$\begin{aligned}\zeta_1 &= p_1 + 2i\hbar a_1 x_1 + p_2 + 2i\hbar a_2 x_2, \\ \zeta_2 &= p_1 + 2i\hbar a_1 x_1 - p_2 + 2i\hbar a_2 x_2.\end{aligned}\tag{4.55}$$

This operator can be employed to check whether a generic state or at least a state close to stationary solution will evolve towards the stationary one. Since ζ_i satisfies the eigenvalue equation, its variance is zero. For the initial state, ζ_i 's variance must be positive by definition. Therefore localization must occur If for a state the condition

$$M \frac{d(\Delta\zeta_i)^2}{dt} \leq 0 \tag{4.56}$$

is showed to be true. Once the Localization is verified, the rate for Localization can be calculated. Furthermore from the definition (3.10) the density matrix of the system can be recovered.

CHAPTER 5

CONCLUSION

In this study, two main approaches to dynamics of open systems was dwelled upon. The methods can be based either on purely algebraic concepts, or they can be, constructive techniques which are based on physical approximations. The main feature of commonly used axiomatic and constructive schemes is the Markov property. This property puts restrictions on the type of the interaction and environment. As stated earlier, the Markov assumption holds in the weak coupling limit, which enables the application perturbation theory, and the reservoir correlation functions decay in a desired timescale. If there is a strong coupling however, master equation can still be obtained by introducing a time scaling parameter to the interaction Hamiltonian and the Hamiltonian of the environment[10]. The reservoir is assumed to be large so that correlation functions can be approximated as analytic functions of frequency. Hence, they act like $\delta(\tau)$ in the time integrals. The physical approximations in the constructive approach naturally lead to a hierarchy between the timescales. Two types of relation between the timescales were considered which lead to Lindbladian and Caldeira-Leggett master equations.

As an important aspect of Lindblad equation, in section (2.2.2), it was verified that if the reservoir is in thermal equilibrium, the canonical form of ρ_A is the invariant state of the master equation. As time goes to infinity, the reduced density matrix will turn into a canonical ensemble regardless of its initial state. If the system has this property it is said to be *ergodic*. In most non-equilibrium problems in statistical physics the ergodicity is a reasonable assumption from the physical point of view. Mathematically, the ergodic property holds if the system operators satisfy[12]

$$\begin{aligned} [F, \alpha(\omega)] &= [F, \alpha^\dagger(\omega)] \\ &= 0, \end{aligned} \tag{5.1}$$

if and only if F is an operator proportional to identity.

Markov property of Caldeira-Leggett model was ensured for the high temperature limit where noise and dissipation kernels decay in short timescales. This means that

$$\langle \beta_1(0) \beta_1^\dagger(-\tau) \rangle \approx \delta(\tau) \quad (5.2)$$

Taking the fourier transform of both sides gives

$$\lambda(\omega) \sim \lambda_0 \quad (5.3)$$

where λ_0 which is independent of frequency ω , is some constant of the reservoir. On the other hand, the KMS relation is

$$\lambda_{ij}(-\omega) = e^{-\omega\sigma} \lambda_{ji}(\omega) \quad (5.4)$$

In section (2.1.2), the canonical distribution for ρ_A being the stationary state of Lindbladian was verified by the relation above. However in Caldeira Leggett model, KMS relation implies that $\lambda(\omega)$ must depend on ω . Thus, from this point of view, the equilibrium state of Caldeira-Leggett master equation seem problematic[12]. Moreover, (2.115) was cast into Lindblad form by separating the dissipator part which results in the modification of the system Hamiltonian with an anti-commutator of x_i and π_i . The physical interpretation of this term remains rather unclear.

For our model, the stationary solution is found as

$$\psi(x_i) \propto \exp\left(a_i(x_i - \langle x_i \rangle)^2 + \frac{i}{\hbar} \langle p_i \rangle (x_i - \langle x_i \rangle)\right). \quad (5.5)$$

Equation (5.5) indicates that the solution is a gaussian wavefunction centered at $\langle x_i \rangle$. Given the fact that localization property is satisfied, an arbitrary initial state is expected to evolve into stationary solution after a certain time. The solution satisfies the equality in (4.53) suggesting that wavefunction is localized in the phase space and in fact, the solution is a generalized coherent state[20]. This is important since the coherent states are the most classical like states showing quantum coherence. The solution however differs from the real coherent states of the Landau problem.[21]

$$\psi_{coherent} \propto \exp\left(-\frac{m\omega}{4\hbar}((x_i - \langle x_i \rangle)^2 - 2i\epsilon_{ij}x_i\langle x_j \rangle)\right) \quad (5.6)$$

Second term in the exponential can be obtained by applying the exponential of a scalar times the creation operator a^\dagger to the ground state. This implies that the coherent

state is a superposition of states from all Landau levels. It satisfies

$$\sigma(x_i, x_i)\sigma(p_i, p_i) = \frac{\hbar^2}{4}. \quad (5.7)$$

Hence, it has the minimum uncertainty. On the other hand, the stationary solution is more spread in the phase space but still localized. One may infer that through the interaction the density matrix for this model will attain an approximately diagonal form in the phase space. Then this would give an idea about how the classicality emerges as a result of interaction. In this context, the density matrix of the system can be interpreted as[20]

$$\rho = \int dx_i dp_i w(x_i, p_i) |\psi_{x_i, p_i}\rangle \langle \psi_{x_i, p_i}|, \quad (5.8)$$

where $w(x_i, p_i)$ stands for the weight function which shows the population of the stationary states $|\psi_{x_i, p_i}\rangle \langle \psi_{x_i, p_i}|$. For each stationary state, weight function must include the cumulative effect of the terms with order $d\xi$ which corresponds to mean over the possible paths. It is also instructive to see that if the parameters μ and ν go to zero, than the stationary solution becomes a coherent state with an arbitrary center of cyclotron motion.

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