



Turun yliopisto
University of Turku

STOCHASTIC DESCRIPTIONS AND MEMORY EFFECTS IN OPEN SYSTEM DYNAMICS

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The originality of this thesis has been checked in accordance with the University of Turku quality assurance system using the Turnitin OriginalityCheck service.

ISBN 978-951-29-5985-3 (PRINT)

ISBN 978-951-29-5986-0 (PDF)

ISSN 0082-7002

Painosalama Oy - Turku, Finland 2015

Acknowledgments

This Thesis summarizes the work done at the Turku Centre for Quantum Physics at the department for Physics and Astronomy in the University of Turku during the years 2010-2014.

I would like to thank my supervisors Jyrki and Kalle-Antti for sharing their knowledge of physics with me and for providing the correct amount of freedom and guidance during my thesis work. I have enjoyed our discussions tremendously. Furthermore, I would like to thank my co-authors Sabrina, Kari, Barry, Constantinos, Elsi and Pinja for fruitful collaboration.

All the people at the old and new “corridor” have created a very nice working atmosphere. I would like to thank all of you. Especially I would like to thank Sabrina, Otto, Elsi, Pinja and Antti for all the nice memories in and out of office.

I am grateful for Väisälä Foundation and the Department of Physics and Astronomy in the University of Turku for their financial support.

This Thesis also finalizes my ten years of studies of physics in Turku. I would like to thank all my friends for being there and for making these ten years unforgettable.

Finally, I would like to thank my family and especially Essi for making all this possible.

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Abstract

In this thesis, methods for solving non-Markovian dynamics are developed and different aspects of the non-Markovian dynamics are studied. Chapter 1 contains a general introduction and the relevant parts of the theory of open quantum systems are presented in chapters 2 and 3.

In chapter 4 we study the possibility to use classical stochastic processes to simulate the dynamics of open quantum systems. We discuss the different methods suitable for Markovian and non-Markovian dynamics. In the Markovian case the stochastic unraveling has a clear physical interpretation in terms of time continuous quantum measurements. In the non-Markovian case, the unraveling provides additional insight on the non-Markovian dynamics but the physical interpretation of the process is debated.

Chapter 5 is devoted for studying the effects of non-Markovianity in specific physical models and the origin of non-Markovianity in these models. Entanglement trapping is studied in a photonic band gap model. We propose an experimentally realizable method how to detect non-Markovianity of quantum dynamics by continuously measuring only a part of the environment of the open system. We also apply methods developed originally for quantum systems to a classical system.

An experimentally realizable model of non-Markovian quantum random walk is constructed in chapter 6 and in chapter 7 we conclude.

Tiivistelmä

Tässä väitöskirjassa on tutkittu muistiefektien vaikutusta sekä kvantti että klassisten systeemien dynamiikkaan. Lisäksi on kehitetty menetelmiä dynamiikan ratkaisemiseksi kun systeemin dynamiikkaa ei voi kuvata Markovisella teorialla. Kappale 1 sisältää yleisen johdatuksen aihepiiriin. Kappaleissa 2 ja 3 esitellään avoimen kvanttisysteemien teoriaa tämän väitöskirjan kannalta olennaisesta näkökulmasta.

Kappaleessa 4 tutkitaan klassisten stokastisten prosessien käyttämistä avointen kvanttisysteemien dynamiikan simuloimiseen. Erilaisien menetelmien esittelyn lisäksi tarkastellaan muistiefektien vaikutusta stokastisten prosessien fysikaaliseen tulkintaan.

Kappaleessa 5 tutkitaan ei Markovista dynamiikka erilaisissa systeemeissä. Tavoitteena on ymmärtää muistiefektien vaikutus dynamiikkaan sekä miksi Markovinen kuvaus ei toimi esimerkkisysteemeille. Lisäksi tarkastellaan kietoutumisen loukuttumista, muistiefektien kokeellista havainnointia sekä sovelletaan kvanttisysteemeille kehitettyjä menetelmiä klassisiin systeemeihin.

Kappaleessa 6 tutkitaan muistiefektejä kvanttikävelyissä mallilla, joka on myös kokeellisesti toteutettavissa. Kappaleessa 7 esitetään yhteenveto tuloksista.

List of articles

This thesis consists of an introductory review and the following five articles:

- I K. Luoma, K.-A. Suominen, and J. Piilo,
Connecting two jumplike unravelings for non-Markovian open quantum systems,
Phys. Rev. A 85, 032113 (2011) (10 pages).
- II C. Lazarou, K. Luoma, S. Maniscalco, J. Piilo, and B. M. Garraway,
Entanglement trapping in a non-stationary structured reservoir,
Phys. Rev. A 86, 012331 (2012) (9 pages).
- III E.-M. Laine, K. Luoma and J. Piilo,
Local-in-time master equations with memory effects: applicability and interpretation,
J. Phys. B: At. Mol. Opt. Phys. 45, 154004 (2012) (8 pages).
- IV K. Luoma, K. Härkönen, S. Maniscalco, K.-A. Suominen, and J. Piilo,
Non-Markovian waiting-time distribution for quantum jumps in open systems,
Phys. Rev. A 86, 022102 (2012) (8 pages).
- V K. Luoma, P. Haikka and J. Piilo,
Detecting non-Markovianity from continuous monitoring,
Phys. Rev. A 90, 054101 (2014) (4 pages).

Chapter 1

Introduction

Quantum mechanics describes Nature in the atomic scale. The theory contains concepts and predicts phenomena that are very different from our everyday classical experience, such as quantum entanglement or quantum steering [1]. Description of a perfectly isolated quantum system is given by the Schrödinger equation. In reality, the vast majority of quantum systems can never be perfectly isolated, there is always some external environment that interacts with the quantum system. Such systems, that are not closed, are called open.

The interaction with the external environment leads to decoherence and dissipation effects, which are detrimental to the quantum properties, such as entanglement. A fundamental object in the study of open quantum systems is the dynamical map, which is a family of completely positive and trace preserving maps that govern the time evolution of the open quantum system. When the dynamical map satisfies the semigroup condition, the time evolution is defined to be Markovian. The characterization of the structure of the quantum dynamical semigroup is one of the most important results in the theory of open quantum systems [2, 3]. Furthermore, it can be used to model dissipation and decoherence effects in many realistic systems, for example many quantum optical systems are well described by the quantum Markov process, i.e. the quantum dynamical semigroup.

The Markovian dynamics of an open quantum system and the quantum measurement theory are closely connected. Indeed, the dynamics, generated by the dynamical semigroup, can be seen to emerge from the time continuous measurement of the environment of the open quantum system. The effect of the measurement process on a Markovian open quantum system can be described using classical stochastic processes that are also Markovian. The stochastic process also describes the observed out-

comes of the measurement. The state of the open system is unravelled into stochastic trajectories that are conditioned on the measurement outcome and the mean value of the trajectories corresponds to the state that evolves under the dynamical semigroup. This approach provides additional physical intuition on the dephasing and decoherence processes and it is also an efficient numerical tool for solving the dynamics of the open system.

Like the closed quantum system, the Markovian open quantum system is an idealization, which emerges when the dynamics of the open system is observed on a suitably coarse grained time scale. This description is not possible if the open system and the environment are strongly coupled, or if the reservoir is structured or finite. These types of systems need methods that are capable to describe non-Markovian effects.

However, the general characterization for the generator of a physically valid non-Markovian open quantum system dynamics does not exist. Systematic methods for deriving effective and approximate descriptions of open systems that are capable to describe non-Markovian dynamics exist but the validity of the dynamics has to be checked, in every case, separately. Stochastic unravelling methods exist also for non-Markovian dynamics. The different methods are quite varied in terms of their range of applicability. For stochastic trajectories that take values on the Hilbert space of the system, the physical interpretation of a single trajectory is an open question.

The main aim of this Thesis is to study various aspects of non-Markovian dynamics. These aspects are summarized into the following questions that we would like to give at least partial answers. What is the exact meaning of non-Markovianity in the quantum realm? How classical stochastic processes can be used to generate non-Markovian quantum dynamics? What is the physical origin and what kind of physical phenomena are related to non-Markovianity? How the non-Markovianity of quantum dynamics can be detected?

The outline of the thesis is the following. In chapter 2 we review the relevant theoretical tools needed to study open quantum systems. We introduce a few of the various different definitions for quantum non-Markovianity in chapter 3. In chapter 4 we overview different stochastic unraveling methods for both Markovian and non-Markovian open quantum systems. We apply some of these methods to an exactly solvable model of an open quantum system and to a classical non-Markov chain in chapter 5. We study non-Markovianity in a discrete dynamical system in chapter 6 and in chapter 7 we conclude.

Chapter 2

Open quantum systems

In order to discuss an open quantum system one needs the notion of a closed quantum system. Let \mathcal{H}_S denote the Hilbert space of the quantum system of interest and let $|\psi_t\rangle \in \mathcal{H}_S$. $|\psi_t\rangle$ is the (pure) state of the system S. For a closed system the time evolution of the state $|\psi_t\rangle$ is given by the Schrödinger equation [4]

$$\frac{d}{dt}|\psi_t\rangle = -iH(t)|\psi_t\rangle, \quad (2.1)$$

where $H(t)$ is the Hamiltonian operator. In Eq. (2.1) and in the rest of the thesis we use such units that $\hbar = 1$. The solution of Eq. (2.1) is expressed as

$$U_{t,t_0} = T_{\leftarrow} e^{-i \int_{t_0}^t ds H(s)}, \quad (2.2)$$

with $U_{t_0,t_0} = \mathbb{I}$ and where T_{\leftarrow} is chronological time-ordering operator. Operator U_{t,t_0} is a unitary operator. This implies that the purity of the state of the closed quantum system S stays constant during the time evolution.

In reality most quantum systems are not closed since they cannot be perfectly isolated from their surroundings. Indeed, an open quantum system is defined to be a quantum system which is not closed. Mathematical description of an open quantum system should thus take into account decoherence and dissipation effects which are caused by the interaction between the system and the environment. These effects cannot be described by unitary dynamics.

The rest of this chapter is organized the following way. In section 2.1 we discuss the structure of the general state space $\mathcal{S}(\mathcal{H}_S)$ which contains

also mixed states and we define the most general physical dynamics for the elements of $\mathcal{S}(\mathcal{H}_S)$. In section 2.2 we discuss the well known case of Markovian open quantum systems and in section 2.3 we overview some approaches that can be used to study situations where the Markovian description fails.

2.1 Quantum dynamical map

States of a quantum mechanical system are generally described by positive trace class operators of unit trace [5]

$$\mathcal{S}(\mathcal{H}) = \{\rho \mid \rho \geq 0, \text{tr} \{\rho\} = 1\}. \quad (2.3)$$

A bounded operator T acting on some Hilbert space is in trace class if the trace of $|T|$ is finite [6]. Since a density matrix ρ is positive it is also self-adjoint and has a spectral decomposition: $\rho = \sum_k \lambda_k |\phi_k\rangle\langle\phi_k|$, where $\lambda_k > 0$ and $\sum_k \lambda_k = 1$. There are uncountably many ways to express ρ as a convex combination. Extremal elements of $\mathcal{S}(\mathcal{H})$ are rank-1 projectors which correspond to pure states.

In order to describe the interaction of the open quantum system S with its environment E we need to work with the following extended Hilbert space $\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_E$, where $\mathcal{H}_S, \mathcal{H}_E$ are the Hilbert spaces of the system and the environment, respectively. Usually the environment is much larger than the system in the sense of Hilbert space dimensions. From now on \mathcal{H} is understood as the Hilbert space of the composite system $S + E$.

Dynamics of the open quantum system can be thought of as a mapping $\Phi_t : \mathcal{S}(\mathcal{H}_S) \rightarrow \mathcal{S}(\mathcal{H}_S)$. A valid mapping Φ_t must be

1. completely positive (CP),
2. trace preserving (TP).

Trace preservation follows from the fact that valid states must have unit trace. Complete positivity guarantees that the positive operators acting on $\mathcal{H}_S \otimes \mathcal{H}_A$ are mapped into positive operators when the map is extended as $\Phi_t \otimes \mathbb{I}_A$, where A is an arbitrarily large ancilla. When $\Phi_t \otimes \mathbb{I}_A$ is viewed as an operation acting on two widely separated and non-interacting systems, complete positivity guarantees that the states of the composite system $S+A$ are mapped into states. We want to represent the map Φ_t only in terms of operators acting on \mathcal{H}_S .

The following is the standard approach to construct a valid dynamical map for the open quantum system which is presented schematically in

$$\begin{array}{ccc}
\varrho(0) = \rho_S(0) \otimes \rho_E & \xrightarrow{\text{unitary evolution}} & \varrho(t) = U_t \rho_S(0) \otimes \rho_E (U_t)^\dagger \\
\downarrow \text{tr}_E & & \downarrow \text{tr}_E \\
\rho_S(0) & \xrightarrow{\text{dynamical map } \Phi_t} & \rho_S(t)
\end{array}$$

Figure 2.1: Schematic construction of dynamical map.

Fig. 2.1. First we need to be able to prepare the system and the environment initially into a product state $\varrho(0) = \rho_S(0) \otimes \rho_E$, secondly we need the dynamics of the composite (S + E)-system (which is considered to be closed), $U_t = U(t, 0) = e^{-iHt}$, where

$$H = H_S \otimes \mathbb{I}_E + \mathbb{I}_S \otimes H_E + H_I \quad (2.4)$$

is the Hamiltonian (time independent, for simplicity) for the combined system. Finally we need to remove the environment degrees of freedom from the description by partial trace. This construction defines a family of CPTP maps Φ_t as

$$\rho_S(t) = \Phi_t \rho_S(0) = \text{tr}_E \left\{ U_t (\rho_S(0) \otimes \rho_E) U_t^\dagger \right\}. \quad (2.5)$$

Stinespring's dilation theorem states that all CPTP maps can be constructed this way [7].

This approach, although general, lacks physical intuition and is in most cases overly complicated since we basically need to solve the dynamics of the system of interest and the environment.

2.2 Markovian open quantum systems

When a dynamical map Φ_t , defined in Eq. (2.5), satisfies the semigroup condition

$$\Phi_{t_1+t_2} = \Phi_{t_1} \Phi_{t_2}, \quad t_1, t_2 \geq 0, \quad (2.6)$$

then Φ_t is called a quantum dynamical semigroup or a quantum Markov process. Dynamical semigroup is time-homogeneous. Celebrated theorem by Gorini, Kossakowski and Sudarshan [2] and independently by Lindblad

[3] states that the quantum dynamical semigroup can be presented in exponential form $\Phi_t = e^{\mathcal{L}t}$, which yields that the reduced state of the open system $\rho(t)$ satisfies $\frac{d}{dt}\rho(t) = \mathcal{L}\rho(t)$. Remarkably this theorem also gives a specific form for the generator \mathcal{L}

$$\frac{d}{dt}\rho(t) = -i[H_S, \rho(t)] + \sum_k \gamma_k \left(C_k \rho(t) C_k^\dagger - \frac{1}{2} \{C_k^\dagger C_k, \rho(t)\} \right), \quad (2.7)$$

where C_k are bounded operators acting on \mathcal{H}_S , they are sometimes called Lindblad- or jump operators. On the right hand side, the commutator part describes the coherent evolution with Hamiltonian H and the latter part describes dephasing and decoherence effects. It is worth mentioning that H_S in Eq. (2.7) is not generally the same H_S as in Eq. (2.4).

It is possible that in some physical situations of interest we are faced with a two parameter family of CPTP maps Φ_{t_2, t_1} . This can happen for example if the total Hamiltonian is time dependent. If Φ_{t_2, t_1} satisfies the CP-divisibility condition

$$\Phi_{t_2, t_0} = \Phi_{t_2, t_1} \Phi_{t_1, t_0}, \quad t_2 \geq t_1 \geq t_0 \geq 0, \quad (2.8)$$

where all the maps are CPTP, then the two parameter family is generated by a time dependent generator \mathcal{L}_t which has the same structure as \mathcal{L} in Eq. (2.7) except that $H_S \rightarrow H_S(t)$, $\gamma_k \rightarrow \gamma_k(t)$ and $\gamma_k(t) \geq 0, \forall t, k$. In this case the dynamical map is time-inhomogeneous. Φ_{t_2, t_1} satisfying Eq. (2.8) is called a time-dependent Markovian quantum process [8, 9, 10]

It is widely accepted that dynamical maps satisfying either one of the decomposition conditions (2.6), (2.8) describes memoryless i.e. Markovian, dynamics. If the dynamical map does not satisfy these conditions, the dynamics of the open quantum system obviously deviates from the Markovian or time-dependent Markovian dynamics, but there are many different definitions of non-Markovianity in the quantum realm. Some of these definitions are discussed in Chap. 3. It is usually very difficult to obtain tractable expressions for the dynamical map. Usually, it is easier to try to obtain some approximate form for the generator and in the Markovian, or time-dependent Markovian case, the GKSL-structure in Eq. (2.7) guarantees that the generator produces physically valid dynamics. If the approximations leading to Markovian dynamics cannot be made, then there is no guarantee that the generator is physically valid. In the next section we discuss general methods for obtaining expressions for the generator.

2.3 Non-Markovian open quantum system

In the context of open quantum systems, where a small system S is interacting with a larger environment E , it is very important to search for efficient mathematical descriptions in terms of small set of relevant dynamical variables. The set of dynamical variables must be chosen in a way that they contain enough information to construct the dynamics for the open system S . Projection superoperators, first introduced by Nakajima, Zwanzig and Mori [11, 12, 13], formulate this idea in a precise mathematical way.

A projection superoperator \mathcal{P} is defined to be a linear map $A \mapsto \mathcal{P}A$, where A is an operator acting on \mathcal{H} . It is a projection $\mathcal{P}^2 = \mathcal{P}$. Intuitively, \mathcal{P} needs to be at least positive and trace preserving in order to map any state to a valid physical state, ie. $\rho \in \mathcal{S}(\mathcal{H}) \implies \mathcal{P}\rho \in \mathcal{S}(\mathcal{H})$. In the context of open quantum systems we also want $\rho_S = \text{tr}_E \{\rho\} = \text{tr}_E \{\mathcal{P}\rho\}$. An interesting class of projection superoperators satisfying all these conditions are introduced in [14, 15], where instead of positivity, complete positivity is required. In [14] it is shown, that the GKSL theorem can be generalized by using correlated projection superoperators.

In the standard approach, the projection superoperator is taken to be $\mathcal{P}\rho = \text{tr}_E \{\rho\} \otimes \rho_E$, where ρ_E is a stationary state of the environment. In this thesis we limit ourselves to the standard choice. Our aim is to derive an equation of motion for the relevant part $\mathcal{P}\rho$, and there are two different approaches that are relevant in the scope of this thesis. With the methods presented in the next two subsections, one can derive generators for dynamical maps that do not have semigroup (2.6) or CP-divisibility (2.8) properties. For the rest of this chapter we work in the interaction picture.

2.3.1 Nakajima-Zwanzig projection operator method

With the initial condition $\mathcal{P}\rho(0) = \rho(0)$, after introducing complementary projection by action $\mathcal{Q}\rho = \rho - \mathcal{P}\rho$ and assuming that odd moments of $H_I(t)$ with respect to the reference state ρ_E vanish, general form for the Nakajima-Zwanzig (NZ) master equation is

$$\frac{d}{dt}\mathcal{P}\rho(t) = \int_{t_0}^t ds \mathcal{K}(t, s)\mathcal{P}\rho(s), \quad (2.9)$$

where $\mathcal{K}(t, s) = \alpha^2 \mathcal{P}\mathcal{W}(t)\mathcal{G}(t, s)\mathcal{Q}\mathcal{W}(s)\mathcal{P}$ is called the memory kernel, $\mathcal{G}(t, s) = T_{\leftarrow} e^{\alpha \int_s^t ds' \mathcal{Q}\mathcal{W}(s')}$ and $\mathcal{W}(t)A = -i\alpha[H_I(t), A]$, for any operator

A acting on \mathcal{H} [9]. This equation is exact but solving this equation is as complicated as solving the complete S + E dynamics. Systematic approximation of the NZ master equation is provided by expanding the memory kernel $\mathcal{K}(t, s)$ in the coupling strength [16].

2.3.2 Time-convolutionless projection operator method

NZ-master equation contains integration over a memory kernel, which is a superoperator itself. This is by no means simple. Time-convolutionless (TCL) approach circumvents this problem by providing a local in time master equation for the relevant part

$$\frac{d}{dt}\mathcal{P}\rho(t) = \mathcal{K}(t)\mathcal{P}\rho(t), \quad (2.10)$$

which is again exact. Derivation of this is very complicated and the details can be found in [9]. The basic idea is to introduce a formal backward propagator in the NZ equations, which can be used to express the relevant part at times $s < t$ in terms of $\mathcal{P}\rho(t)$. Solving the exact equation is again essentially as complicated as solving the full S + E dynamics. Again, there exists a systematic perturbation expansion in the coupling strength for the generator $\mathcal{K}(t)$. For example, the second order generator (TCL2) takes the form

$$\mathcal{K}_2(t) = \int_{t_0}^t ds \mathcal{P}\mathcal{W}(t)\mathcal{W}(s)\mathcal{P}. \quad (2.11)$$

By requiring that $\text{tr}\{\mathcal{P}\rho(t)\} = 1$ and $\mathcal{P}\rho(t) = \mathcal{P}\rho(t)^\dagger$ for all times t , it can be shown that the TCL generator in any order must be of the following general form [17]

$$\mathcal{K}(t)\mathcal{P}\rho(t) = -i[H_{\text{TCL}}, \mathcal{P}\rho(t)] + \sum_k \gamma_k(t) \left(C_k \mathcal{P}\rho(t) C_k^\dagger - \frac{1}{2} \{C_k^\dagger C_k, \mathcal{P}\rho(t)\} \right). \quad (2.12)$$

In literature, this form is sometimes referred to as the time-dependent Lindblad-form. We refer to this form as the time-dependent GKSL-form.

Starting from the TCL2 generator in Eq. (2.11) and with the standard projection superoperator one can do further approximations, that are usually valid in quantum optical systems, which lead to a quantum dynamical

semigroup. To get a time independent description, let the integration limit go to infinity. This is justified if the time scale for the decay of correlations between the system and environment (τ_C) is much smaller than the relaxation time scale for the system (τ_R), i.e. $\tau_R \gg \tau_C$. In order to get the GKSL-form, rapidly oscillating terms need to be neglected. This can be done if the typical time scale of the system (τ_S), defined by inverse value of typical energy level separation of the system, is smaller than the relaxation time scale τ_R .

Chapter 3

Measures for quantum non-Markovianity

A classical Markovian stochastic process has a very precise definition, which is expressed in terms of the conditional transition probabilities for the process. For a stochastic process $\{x_n\}_{n \in \mathbb{Z}_+}$ taking values in a countable set, it is stated as

$$p_{1|n}(x_n, t_n | x_{n-1}, t_{n-1}; \dots; x_0, t_0) = p_{1|1}(x_n, t_n | x_{n-1}, t_{n-1}). \quad (3.1)$$

for $t_n \geq t_{n-1} \geq \dots \geq t_0$. The condition says that the probability to find the process in a state x_n at time t_n depends only on its state at time t_{n-1} . Stochastic processes fulfilling the Markov condition also satisfy the Chapman-Kolmogorov equation [9]

$$p_{1|1}(x_3, t_3 | x_1, t_1) = \sum_{x_2} p_{1|1}(x_3, t_3 | x_2, t_2) p_{1|1}(x_2, t_2 | x_1, t_1), \quad (3.2)$$

which is an equation for the conditional probabilities $p_{1|1}(\cdot|\cdot)$ [18]. The classical Markov condition can not be transferred to the quantum realm because the notion of conditional probability depends on the measurement required to discern the previous value of the random variable and on how the measurement transforms the state for future evolution [19].

These difficulties have led to different characterizations of quantum non-Markovianity. First of all, it would be desirable that a quantity measuring non-Markovianity of a quantum system is at least computable, unitarily invariant, experimentally realizable and has a physical interpretation [20, 21].

In [20] Markovianity or non-Markovianity of a quantum channel describing the time evolution of an open quantum system is assessed from the

structure of the map at a single instant of time. The assessment criteria can be turned into a measure for non-Markovianity if one measures how much isotropic noise has to be added into the channel for it to become a semi-group. Another proposal for defining non-Markovianity based on structural properties of quantum channels is in [22]. This measure quantifies indivisibility of a quantum dynamical map (2.8) by measuring the violations of complete positivity of the map Φ_{t_2, t_1} . Recent proposal in [23] establishes a formal analogy between the entanglement theory and quantum evolutions by introducing a degree for non-Markovianity. Various other approaches are based on quantum Fisher information flow [24], fidelity [25], mutual information [26], channel capacity [21], geometry of the set of accessible states [27] and distinguishability between quantum states [8].

In this thesis we focus on the last proposal. This measure for non-Markovianity is based on the fact that under CPTP-maps^a, the trace distance between two quantum states decreases [29]. The quantity

$$\sigma(\rho_1, \rho_2, t) = \frac{d}{dt} \|\Phi_t(\rho_1 - \rho_2)\|_1, \quad (3.3)$$

where $\|\cdot\|_1$ is the trace norm, and ρ_k , $k = 1, 2$ are two initial states of the system S , is interpreted as information flow. When $\sigma(\rho_1, \rho_2, t) \leq 0$, information flows from the system to the environment and when $\sigma(\rho_1, \rho_2, t) > 0$ there is a backflow of information from the environment to the system. For a Markovian system (CP-divisible) the information flows always from the system to the environment, $\sigma(\rho_1, \rho_2, t) \leq 0$, for all times t and for all pairs of initial states. However, the dynamical map might be indivisible but the backflow of information does not necessarily occur [30, 31]. The measure for non-Markovianity is defined as

$$\mathcal{N}(\Phi) = \max_{\rho_{1,2}} \int_{\sigma > 0} ds \sigma(\rho_1, \rho_2, s) \quad (3.4)$$

This measure contains maximization over all possible pairs of initial states. It has been shown that the maximization of $\mathcal{N}(\Phi)$ can be restricted to orthogonal state pairs [32] or equivalently over an enclosing surface around a fixed state belonging to the interior of the state space $\mathcal{S}(\mathcal{H}_S)$ [33]. This measure is chosen because it has a clear physical interpretation in terms of information flow. Quantum process tomography is not needed, since the

^aActually, all positive trace preserving maps are contractive with respect to the trace norm [28].

measure is computed from the evolution of a pair of quantum states and this measure is also experimentally realizable [34].

It should be noted that the different measures for non-Markovianity are generally incompatible with each other [19]. Also, it would be very important to find some operational meaning for non-Markovianity. Some steps towards this direction have been taken in [35, 21] where non-Markovianity is used as a resource for quantum information tasks.

Chapter 4

Stochastic methods for open quantum systems

As we have discussed earlier, a general state of a quantum system S is described by a density matrix ρ . It is clear that when the size of the system grows, solving the dynamics for the reduced system becomes increasingly more complicated. There exists an alternative way of solving the dynamics of an open quantum system by evolving only pure states, which is computationally less demanding. This is done by defining a \mathcal{H}_S valued stochastic process which amounts to defining a probability density functional $P[\psi]$ on the projective Hilbert space $\mathcal{P}(\mathcal{H})$. In projective Hilbert space, states that differ only by a global phase factor belong to the same equivalence class, e.g. $|\phi\rangle \sim e^{i\theta}|\phi\rangle$. By using the probability density, the density matrix is written as

$$\rho = \mathbb{E} [|\psi\rangle\langle\psi|] = \int d\psi P[\psi] |\psi\rangle\langle\psi|, \quad (4.1)$$

where $d\psi \equiv d\psi d\psi^*$ is a functional volume element [36].

Time evolution of the probability density $P[\psi, t]$ thus defines the evolution of the open quantum system completely. There are many different probability density functionals corresponding to the same state $\rho_S(t)$. In this sense, $P[\psi, t]$ contains more information than the density matrix itself. From a statistical ensemble of pure states $\{\psi_i(t)\}_{i=1}^N$ the probability density is estimated as $P[\phi, t] = \sum_{\alpha} \frac{N_{\alpha}}{N} \delta[\phi - \psi_{\alpha}]$, where N_{α} is the number of states in the ensemble that belong to the same equivalence class and $\delta[\phi - \psi]$ is a functional that satisfies $\int d\phi \delta[\psi - \phi] F[\phi] = F[\psi]$ for an arbitrary smooth functional F and $\int d\psi \delta[\psi - \phi] = 1$.

Using Eq. (4.1) we find that $\rho_S(t) = \frac{1}{N} \sum_{\alpha} N_{\alpha} |\psi_{\alpha}(t)\rangle\langle\psi_{\alpha}(t)|$. Standard deviation measures the error of the finite sampling and it scales with the inverse square root of the sample size N . Roughly, the stochastic methods can be divided into two categories; into diffusion- and piecewise deterministic processes.

In this chapter we will discuss different stochastic processes which can be used to solve Markovian and non-Markovian dynamics. We also discuss how methods suitable for Markovian dynamics might be used to solve non-Markovian dynamics by embedding the system of interest into a larger system which obeys Markovian dynamics.

4.1 Methods for Markovian open systems

4.1.1 Piecewise deterministic processes

Any master equation in the GKSL or the time-dependent GKSL form of Eq. (2.7) can be unravelled by the following Ito stochastic differential equation [9]

$$d\psi(t) = -iG(\psi(t))dt + \sum_i \left(\frac{C_i\psi(t)}{\|C_i\psi\|} - \psi(t) \right) dN_i(t), \quad (4.2)$$

where $G(\psi(t)) = H\psi(t) - \frac{i}{2} \sum_k \gamma_k(t) \left(C_k^\dagger C_k \psi(t) - \|C_k\psi(t)\|^2 C_k \psi(t) \right)$ and Poisson increments $dN_i(t)$ satisfy

$$dN_i(t)dN_j(t) = \delta_{ij}dN_j(t), \quad (4.3)$$

$$\mathbb{E}[dN_i(t)] = \gamma_i(t) \|C_i\psi(t)\|^2 dt. \quad (4.4)$$

It is easy to show that the time evolution of a priori state $\rho(t) = \mathbb{E}[|\psi(t)\rangle\langle\psi(t)|]$ is generated by the GKSL master equation.

Sample paths of the process consist of two different types of evolutions; if $dN_i(t) = 0 \forall i$ then $\psi(t)$ evolves continuously with $\frac{d}{dt}\psi(t) = -iG(\psi(t))$, if $dN_i(t) = 1$ then $dN_{i \neq k}(t) = 0$ and $\psi(t)$ evolves discontinuously and instantaneously to $\psi(t) \mapsto \frac{C_i\psi(t)}{\|C_i\psi(t)\|}$. The norm of $\psi(t)$ is conserved during both types of evolution. The operator

$$H_{\text{eff}}(t) = H - \frac{i}{2} \sum_k \gamma_k(t) C_k^\dagger C_k \quad (4.5)$$

is called an effective Hamiltonian which is non-Hermitian. This type of stochastic state vector evolution was first introduced to describe quantum optical systems [37, 38, 39, 40, 41, 42, 43]. A different approach in terms of a classical Markov process in projective Hilbert space, leading to same type of a stochastic process for state vectors can be found in [44, 36, 45].

There are two different types of algorithms that can be used to generate sample paths of the process. First one evolves the stochastic state vector in stepwise fashion [37]. Let $U_{t+\delta t,t} \approx (\mathbb{I} - i\delta t H_{\text{eff}}(t))$ and let $\rho(t) = \int d\psi P[\psi, t] |\psi\rangle\langle\psi| = \frac{1}{N} \sum_{i=1}^N |\psi_i(t)\rangle\langle\psi_i(t)|$. We present the algorithm for a single ensemble member $\psi_i(t)$.

1. Calculate the jump probability densities

$$P_k[\phi|\psi_i(t)] = \delta t \gamma_k(t) \|C_k \psi_i(t)\|^2 \delta[\phi - \frac{C_k \psi_i(t)}{\|C_k \psi_i(t)\|}].$$
2. Choose a uniformly distributed random number $\eta \in [0, 1]$.
 - (a) If $1 - \int d\phi \sum_k P_k[\phi|\psi_i(t)] > \eta$, then $\psi_i(t) \mapsto \psi_i(t + \delta t) = \frac{U_{t+\delta t,t} \psi(t)}{\|U_{t+\delta t,t} \psi(t)\|}$
 - (b) If $1 - \int d\phi \sum_k P_k[\phi|\psi_i(t)] < \eta$, then $\psi_i(t) \mapsto \psi_i(t + \delta t) = \frac{C_k \psi_i(t)}{\|C_k \psi_i(t)\|}$
with probability $\frac{\int d\phi P_k[\phi|\psi_i(t)]}{\int d\phi' \sum_k P_k[\phi'|\psi_i(t)]}$.

This algorithm produces, for a single sample path, either continuous or a discontinuous evolution over the time interval δt . Sometimes this is referred to as the Monte Carlo Wave Function (MCWF) method.

Another algorithm to evolve stochastic state vector is to sample the length of the deterministic evolution period from the waiting time distribution (WTD) $F(\tau|\psi, T)$ by solving an implicit equation $F(\tau|\psi, T) = \eta$, where $\eta \in [0, 1]$ is uniformly distributed random number [42, 9]. For a single realization $\psi_i(t)$, the stochastic evolution is the following:

1. Sample η .
2. Solve τ from $F(\tau|\psi_i(t), t) = \eta$.
3. Solve $\frac{d}{ds} \psi_i(s) = G(\psi_i(s))$ on the interval $[t, t + \tau]$.
4. Calculate the jump probability densities $P_k[\phi|\psi_i(t + \tau)]$ and jump $\psi_i(t + \tau) \mapsto \psi_i(t + \tau) = \frac{C_k \psi_i(t + \tau)}{\|C_k \psi_i(t + \tau)\|}$ with probability $\frac{\int d\phi P_k[\phi|\psi_i(t + \tau)]}{\int d\phi' \sum_k P_k[\phi'|\psi_i(t + \tau)]}$.

This algorithm is more accurate since the integration over the deterministic period can be done adaptively. For Markovian dynamics we have a particularly simple form for the WTD

$$F(\tau|\psi, t) = 1 - \|e^{-iH_{\text{eff}}(t+\tau)}\psi(t)\|^2. \quad (4.6)$$

It is important to notice that each sample path is independent, which means that the whole future evolution of a particular sample path can be obtained independently of others.

4.1.2 Quantum state diffusion

Quantum state diffusion refers to a stochastic process where realizations are everywhere continuous but nowhere differentiable. In the Markovian case noise processes driving the system are Wiener processes. The stochastic Ito differential equation takes the following form [46, 47, 48]

$$d\psi(t) = -iG(\psi(t)) + \sum_k \sqrt{\gamma_k(t)} (C_k - \langle C_k \rangle_\psi) \psi(t) dW_k, \quad (4.7)$$

where we have used the following notation: $\langle A \rangle_\psi = \langle \psi|A|\psi \rangle$, $G(\psi) = H\psi + \frac{i}{2} \sum_k \gamma_k(t) \left(2\langle C_k^\dagger \rangle_\psi C_k - C_k^\dagger C_k - \langle C_k \rangle_\psi \langle C_k \rangle_\psi \right) dt$. Wiener process increments satisfy $\mathbb{E}[dW_k] = 0$, $\mathbb{E}[dW_k dW_l] = 0$ and $\mathbb{E}[dW_k^* dW_l] = \delta_{kl} dt$. These types of models were first introduced in the context of stochastic collapse theories [49, 50, 51], where decoherence is not caused by interaction with an external environment. Methods for solving these types of equations can be found in [9, 52]. Here we present the simplest one, namely the Euler-Maruyama method. Consider a SDE of the form $dX = a(X_t)dt + b(X_t)dW$, with the initial condition $X_0 = x_0$ and let $t_0 < t_1 < \dots < t_N = T$ denote a partition of the interval $[0, T]$ into equal sub-intervals with width $\delta t = T/N > 0$. Then the Euler-Maruyama method provides a solution recursively

$$X_{n+1} = X_n + a(X_n)\delta t + b(X_n)\Delta W_n, \quad (4.8)$$

where ΔW_n are independent and identically distributed normal random variables with zero mean and variance δt .

4.1.3 Physical interpretation for Markovian stochastic methods

Remarkably, a physical interpretation for single realizations of stochastic Schrödinger equations of both types can be given. Stochastic pure state

evolutions can be interpreted as conditional trajectories of the open system conditioned on a measurement record obtained from continuous monitoring of the environment. With this interpretation one can say that Markovian stochastic trajectories are subjectively real. Recently, experimental tests were proposed that would rigorously prove that the stochastic evolution of a Markovian open quantum system is detector dependent [53]. There are multiple different approaches on how to derive the stochastic equations from continuous monitoring of the environment.

For a PDP process, an interesting approach is in [36, 44]. The authors construct a Markovian process for a probability density $P[\psi, t]$ in a projective Hilbert space. In this approach the Markov approximation is made on the conditional transition probability or the propagator, $T[\psi, t|\varphi, t]$, such that it satisfies the differential Chapman-Kolmogorov equation, which is a necessary condition for the process to be Markovian. In subsequent work [54] it is shown, how continuous projective measurement of the environment gives rise to this construction. Actually, each application of the Chapman-Kolmogorov equation gives rise to state reduction by some fixed measurement scheme. Authors also show what kind of a measurement scheme gives rise to a diffusive SSE and how diffusion limit is performed on a PDP. For a quantum optical open system, PDP can be interpreted in terms of direct photo detection in the following way. Deterministic periods of evolution correspond to sequences of measurements that yield null outcome. Jumps correspond then to detection of a photon in the environment. In Fig. 4.1 we show an example of a conditional trajectory of a classically driven damped two level atom monitored by direct photo detection [55].

Diffusive SSE in Eq. (4.7) corresponds to stochastic dynamics of heterodyne photo detection in the diffusion limit [9, 55]. Another type of diffusive SSE can be obtained when the environment is monitored by using homodyne detection [55]

$$d\psi(t) = -iK(\psi(t))dt + \sum_k \sqrt{\gamma_k(t)} \left(C_k - \frac{1}{2} \langle C_k + C_k^\dagger \rangle_\psi \right) dW_k, \quad (4.9)$$

where dW_k is a standard real valued Wiener process increment and $K(\psi(t)) = H\psi(t) + \sum_k i\frac{\gamma_k}{2} \left(\langle C_k + C_k^\dagger \rangle_\psi C_k - C_k^\dagger C_k + \frac{1}{4} \langle C_k + C_k^\dagger \rangle_\psi^2 \right) \psi(t)$. During the recent years all diffusive SSE's have been parametrized [56, 57]. In Fig. 4.2 we shown an example of a conditional trajectory of a classically driven damped two level atom monitored by homodyne photo detection[55].

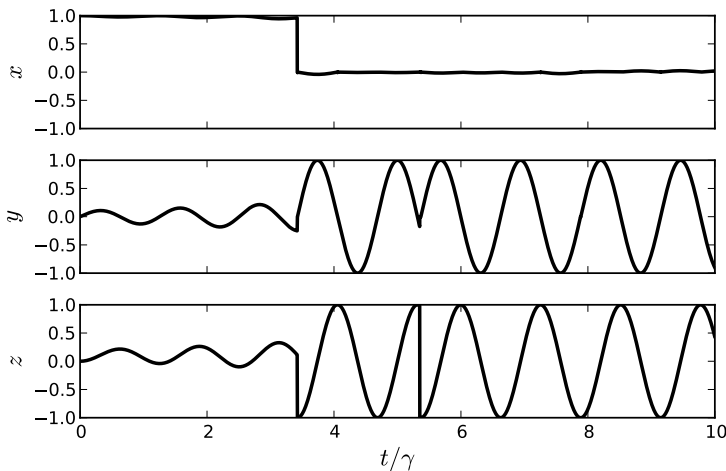


Figure 4.1: Conditional trajectory of a classically driven, damped two level atom monitored with direct photo detection. The trajectory is generated using the stepwise algorithm presented in Sec. 4.1.1

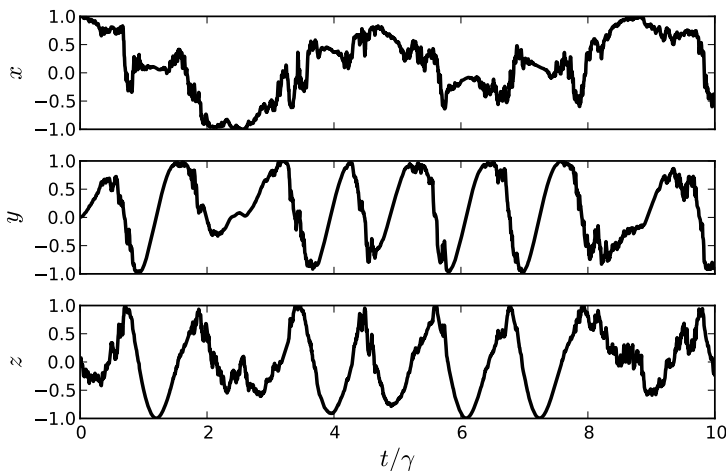


Figure 4.2: Conditional trajectory of a classically driven, damped two level atom monitored with homodyne detection. The trajectory is generated using the Euler-Maruyama method presented in Sec. 4.1.2.

From measurement interpretation perspective it is clear why the ensemble of trajectories contains much more information than the ensemble

average; during the unravelling the measurement record and the state conditioned on the particular measurement record are evolved simultaneously.

4.2 Methods for non-Markovian systems

4.2.1 Non-Markovian quantum jumps

The non-Markovian quantum jump method (NMQJ) in its standard form [58, 59, 60, 61, 62, 63] is a PDP process for state vectors that unravels the following general time local master equation

$$\begin{aligned} \frac{d}{dt}\rho(t) = & -i[H, \rho(t)] + \sum_k \gamma_k^+(t) \left(C_k \rho(t) C_k^\dagger - \frac{1}{2} \{C_k^\dagger C_k, \rho\} \right) \\ & - \sum_l \gamma_l^-(t) \left(C_l \rho(t) C_l^\dagger - \frac{1}{2} \{C_l^\dagger C_l, \rho\} \right), \end{aligned} \quad (4.10)$$

where $\gamma_k^\pm(t) = \frac{1}{2}(|\gamma_k(t)| \pm \gamma_k(t))$ and $\gamma_k^+(t), \gamma_l^-(t) \geq 0$. In Eq. (4.10) there is an overall minus sign in the second summation which makes direct use of stochastic methods developed for Markovian open quantum systems impossible, since a white noise process with negative autocorrelation would be required.

The key idea in the unravelling of Eq. (4.10) into stochastic trajectories is that the negative decay rate leads to a new type of jump that partially restores the coherence lost earlier during the time evolution. Let $P[\psi, t] = \frac{1}{N} \sum_\alpha N_\alpha(t) \delta[\psi - \psi_\alpha(t)]$ and $\rho(t) = \frac{1}{N} \sum_\alpha N_\alpha(t) |\psi_\alpha(t)\rangle \langle \psi_\alpha(t)|$. The tuple $(\{\psi_\alpha\}, \{\frac{N_\alpha(t)}{N}\})$ is called an effective ensemble. It contains a set of states labeled by index α , such that the states with $\alpha \neq \beta$ belong to different equivalence classes and the integers $N_\alpha(t)$ that count the number of ensemble members in state ψ_α . Evolution of the effective ensemble in the NMQJ algorithm over a small time step δt consists of the following components:

1. Deterministic evolution with

$$H_{\text{eff}}(t) = H_S - i \frac{1}{2} \sum_k \gamma_k(t) C_k^\dagger C_k. \quad (4.11)$$

2. Jump probability density for $\psi_\alpha(t) \rightarrow \phi$

$$P_k^+[\phi|\psi_\alpha(t)] = \delta t \gamma_k^+(t) \|C_k \psi_\alpha(t)\|^2 \delta \left[\phi - \frac{C_k \psi_\alpha(t)}{\|C_k \psi_\alpha(t)\|} \right]. \quad (4.12)$$

3. Non-Markovian jump probability density for $\psi_\alpha(t) \rightarrow \phi$

$$P_k^-[\phi|\psi_\alpha(t)] = \delta t \gamma_k^-(t) \frac{P[\phi, t]}{P[\psi_\alpha, t]} \|C_k \phi(t)\|^2 \delta \left[\psi_\alpha(t) - \frac{C_k \phi(t)}{\|C_k \phi(t)\|} \right]. \quad (4.13)$$

Note that 1.) and 2.) are exactly the same as in the MCWF method. 3.) extends NMQJ to regime where $\gamma_k(t)$ may be temporarily negative. It contains a condition that a non-Markovian jump may occur from $\psi_\alpha \rightarrow \phi$ if ϕ is in the support of the jump operator C_k , eg. if

$$\psi_\alpha(t) = \frac{C_k \phi(t)}{\|C_k \phi(t)\|}. \quad (4.14)$$

This condition relates the different sample paths, since during the simulation, state ψ_α is created from a possible target state of a non-Markovian jump ϕ , by an earlier jump via positive decay channel $\gamma_k^+(t)$. This structure also enables the non-Markovian jump to restore coherences. Necessity of this type of structure can be motivated by the following consideration. If C_k has non-empty kernel, only a pseudo inverse operator C_k^+ exists [64]. But this operator is not sufficient because it cannot recover the null space components and is therefore unable to recover all the components (hence also coherences) of the state prior to jump with C_k . However, making the non-Markovian jumps with the condition (4.14), recovers the prior state.

As one can see, the positive jumps build the effective ensemble dynamically and the non-Markovian jumps redistribute the population between the states that are already present in the ensemble. One can define one more quantity, the total jump probability density

$$P_k[\phi|\psi, t] = P_k^+[\phi|\psi, t] + P_k^-[\phi|\psi, t]. \quad (4.15)$$

Usual arguments [9] for deriving the waiting time distribution (WTD) work also for non-Markovian quantum jumps. The result is much more complicated since different sample paths are not independent, see Eq. (4.14). The probability to jump away from $\psi(t)$ during time interval $[t, t + \delta t)$ is $\Gamma[\psi, t] \delta t = \int d\phi \sum_k P_k[\phi|\psi, t]$. The WTD is a conditional probability distribution which gives the probability for the next jump to occur during a time interval $[t, t + \tau)$ conditioned on that the state is known to be ψ at time t . Probability of a jump to occur during a short time interval $[t + \tau, t + \tau + \delta \tau)$ away from ψ is then $\delta F[\tau|\psi, t] = F[\tau + \delta \tau|\psi, t] - F[\tau|\psi, t]$. This is equal to the probability of having no jumps before $T + \tau$ and a jump during the

following $\delta\tau$, i.e., $\delta F[\tau|\psi, t] = (1 - F[\tau|\psi, t])\Gamma[\psi, t + \tau]\delta\tau$. Then dividing by $\delta\tau$ and taking the limit $\delta\tau \rightarrow 0$ we obtain

$$\frac{d}{d\tau}F[\tau|\psi, t] = (1 - F[\tau|\psi, t])\Gamma[\psi, t + \tau]. \quad (4.16)$$

A valid WTD is a solution to Eq. (4.16) with the initial condition $F[0|\psi, t] = 0$. Assuming that $\gamma_k^-(t) = 0, \forall t, k$ then Eq. (4.6) is a solution to Eq. (4.16) if $\|\psi(t)\| = 1$. In paper **IV** we calculated the waiting time distribution explicitly for a few different models and studied the properties of the WTD in terms of those models.

Relation to modal dynamics

In [65] Gambetta, Askerud and Wiseman (GAW) developed a jumplike unravelling for non-Markovian open quantum systems. It is based on the modal interpretation of quantum mechanics [66, 67] where the evolution of the quantum system is expressed in terms of property states. In the context of open quantum systems they are states where some observable of the environment $Z_E = \sum_k z_k \pi_k, \pi_k \pi_l = \delta_{k,l} \pi_k$ has a definite value. For example, the property state corresponding to a value z_k is $|\Psi_{z_k}(t)\rangle = \frac{1}{\sqrt{N_k}} I \otimes \pi_k |\Psi(t)\rangle = \frac{1}{\sqrt{N_k}} |\phi_k(t)\rangle \otimes |z_k\rangle$, where $\pi_k = |z_k\rangle\langle z_k|$ and $|\Psi(t)\rangle \in \mathcal{H}_S \otimes \mathcal{H}_E$. It is then said that in a state $|\Psi_{z_n}\rangle$, the property Z_E has a value z_n .

The modal dynamics (the stochastic evolution between different property states) is given by

$$\frac{dP(z_n, t)}{dt} = \sum_m J_{nm}(t), \quad (4.17)$$

where $J_{nm}(t)$ is the probability current and $P(z_n, t)$ is the probability that the property has the value z_n at time t . The probability current $J_{nm}(t)$ is defined as

$$J_{nm}(t) = \sum_m (T_{nm}(t)P(z_m, t) - T_{mn}(t)P(z_n, t)), \quad (4.18)$$

where $T_{nm}(t)$ are the transition rates from the property state z_m to z_n . The probability current satisfies $J_{mn}(t) = -J_{nm}(t)$. One possible definition for the transition rates that satisfy Eq. (4.17) is the following.

For $J_{nm}(t) < 0$

$$\begin{aligned} T_{nm}(t) &= 0, \\ T_{mn}(t) &= -\frac{J_{nm}(t)}{P(z_n, t)}, \end{aligned} \quad (4.19)$$

and for $J_{mn}(t) > 0$

$$\begin{aligned} T_{mn}(t) &= \frac{J_{mn}(t)}{P(z_m, t)}, \\ T_{nm}(t) &= 0. \end{aligned} \quad (4.20)$$

The probability rule is fixed to be

$$P(z_n, t) = \langle \Psi(t) | \pi_n | \Psi(t) \rangle. \quad (4.21)$$

The probability current can then be calculated using the Schrödinger equation and Eqs. (4.17), (4.21).

It is important to note that in Eq. (4.19) when the probability current for a transition $z_m \rightarrow z_n$ is negative, only the reverse transition $z_n \rightarrow z_m$ may occur and that the rate of the transitions is inversely proportional to the probability $P(z_n, t)$. Comparing this to the non-Markovian jump probability density in Eq. (4.13) we see that it is also inversely proportional to the population in the source state of the jump. In paper **I** we explored how the NMQJ and the GAW methods are related by studying few example systems.

4.2.2 Non-Markovian quantum state diffusion

Non-Markovian quantum state diffusion is a generalization of the quantum state diffusion method to the non-Markovian regime [68, 69, 70, 71]. Given the following Hamiltonian

$$H = H_S + \sum_{\lambda} \left(g_{\lambda} L \otimes a_{\lambda}^{\dagger} + g_{\lambda}^* L^{\dagger} \otimes a_{\lambda} \right) + \sum_{\lambda} \omega_{\lambda} a_{\lambda}^{\dagger} a_{\lambda}, \quad (4.22)$$

for the open quantum system and the environment, then the exact dynamics for the system can be obtained from the following linear stochastic differential equation

$$\partial_t \tilde{\psi}_t[z^*] = -i H_S \tilde{\psi}_t[z^*] + L \tilde{\psi}_t[z^*] z_t^* - L^{\dagger} \int_0^t ds \alpha(t, s) \frac{\delta \tilde{\psi}_t[z^*]}{\delta z_s^*}, \quad (4.23)$$

where z_t^* is colored complex Gaussian noise with the following statistical properties; $\mathbb{E}[z_t^*] = 0$, $\mathbb{E}[z_t z_s] = 0$, $\mathbb{E}[z_t^* z_s] = \alpha(t, s)$ and in the notation we have signified the fact that the stochastic vector is a functional of the noise process. $\alpha(t, s) = \alpha^*(s, t)$ is the environment correlation function

$$a(t, s) = \sum_{\lambda} |g_{\lambda}|^2 e^{-i\omega_{\lambda}(t-s)}. \quad (4.24)$$

We have restricted ourselves to a zero temperature environment, but this is not a limitation of the method. Functional derivative under the integral signifies that the evolution of the state depends on the earlier values of the noise. This equation does not preserve the norm of individual sample paths but the norm is conserved on average, e.g. $\mathbb{E}[|\tilde{\psi}_t[z^*]|] = 1$. It is also possible to define a non-linear version of Eq. (4.23) which preserves the norm along each realization.

These equations, linear and non-linear versions, are very difficult to solve even numerically because of the functional derivative term. In some cases it is possible to use the following ansatz: $\frac{\delta \tilde{\psi}_t[z^*]}{\delta z_s^*} = O(t, s, z^*) \tilde{\psi}_t[z^*]$. The time- and the noise dependence of $O(t, s, z^*)$ can be determined from the consistency condition $\frac{\delta}{\delta z_s^*} \partial_t \tilde{\psi}_t[z^*] = \partial_t \frac{\delta \tilde{\psi}_t[z^*]}{\delta z_s^*}$. If a simple ansatz for the functional derivative can not be found one can try to use different perturbation expansions in order to calculate the ansatz operator $O(t, s, z^*)$ [72]. Perturbation approach allows one to use non-Markovian QSD also for the derivation of approximate master equations for the open system. A recent interesting approach in making non-Markovian QSD more tractable is the hierarchy of pure states state (HOPS) method, where the difficult non-local in time term in Eq. (4.23) is replaced with an auxiliary pure state, and a hierarchy of equations of motion is constructed [73]. Interestingly, by using linear and non-linear NMQSD equations a necessary criterion for the measurement scheme interpretation for the stochastic sample paths is derived in [74].

4.2.3 Pseudomodes

The method of pseudomodes provides a way to map a generally non-Markovian system into a larger Markovian system [75, 76, 77]. In this method the poles of the spectral density

$$J(\omega) = \sum_{\lambda} |g_{\lambda}|^2 \delta(\omega - \omega_{\lambda}), \quad (4.25)$$

in the continuum limit are mapped to fictitious modes, pseudomodes. Dynamics of the open quantum system and the pseudomodes is given by a GKSL-master equation. State of the open system is obtained from the extended system by tracing over the pseudomode degrees of freedom.

This method provides an exact equation without any approximations. However, this method is most efficient when there is in total one excitation in the system and the environment. Some attempts to generalize this method to the case of multiple excitations have been made in Refs. [78, 79], but in general the treatment of the case of multiple excitations is very complicated. More recently, the pseudomode method has been applied to the calculation of absorption spectra of molecular aggregates [80].

We have applied the pseudomode method in paper **II** to study entanglement trapping in photonic band gap model, see Sec. 5.1.3. This method was also used for studying the experimental detection of non-Markovianity of the dynamics of a two level atom in paper **V**, see Sec. 5.1.4.

4.2.4 Embedding methods

There are several methods, with which a system which may exhibit non-Markovian dynamics, is embedded into a larger system which obeys the GKSL equation of motion. Dynamics of the original system can be deduced from the dynamics of the extended system. The pseudomode method in Sec. 4.2.3 is one example of such an embedding method.

A method closely related to the pseudomode method was introduced in [81]. In this method the spectral density is expressed (approximately or exactly) as a linear combination (with positive coefficients) of Lorentzians. Each Lorentzian corresponds to a fictitious harmonic oscillator mode. The original system is coupled coherently to fictitious modes and the fictitious modes are coupled to external environment in such a way that the extended dynamics obeys the GKSL-master equation. Tracing over the fictitious modes gives the solution of the original problem. The pseudomode method can be seen as a generalization of this approach since it can solve the cases with negative expansion coefficients.

In [82] a method for unravelling the most general type of master equation (2.12) with MCWF-method in extended Hilbert space $\mathcal{H}_S \oplus \mathcal{H}_S$ is developed. The stochastic vector $\theta = (\psi \ \phi)^T \in \mathcal{H} \oplus \mathcal{H}$ is evolved in such a way that the state of the open system is obtained as $\mathbb{E}[|\psi\rangle\langle\phi|]$. This method has a drawback when applied to Eq. (4.10). If there are non-zero negative decay rates, then the norm of the stochastic vector is increas-

ing during the periods of deterministic evolution. A slight modification of this method is presented in [83], where the ensemble average is taken over $\mathbb{E} [|\psi\rangle\langle\phi| + |\phi\rangle\langle\psi|]$. The operator $|\psi\rangle\langle\phi| + |\phi\rangle\langle\psi|$ is Hermitian and it is required that the norm of the operator is conserved along each trajectory.

In [17], yet another embedding is introduced, this time into the enlarged Hilbert space $\mathcal{H}_S \oplus \mathcal{H}_S \oplus \mathcal{H}_S$. Norm of each trajectory is conserved and the reduced state of the open system is obtained as $\rho(t) = \frac{W_{12}}{\text{tr}\{W_{12}\}}$. Here $W(t)$ is the state of the enlarged system, with initial condition $W(0) = \rho(0) \otimes |\chi\rangle\langle\chi|$, where $|\chi\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle)$ and $W_{12}(t) = \langle 1|W(t)|2\rangle$.

Chapter 5

Non-Markovianity in simple quantum and classical systems

In this chapter we study an analytically solvable model of an open quantum system by using some of the methods presented in the earlier chapters. Our open system is a single two level atom that interacts with an environment, namely the electromagnetic field in zero temperature.

We also use the time local master equation formalism on a classical system to study classical non-Markov chains.

5.1 Quantum open system: analytically solvable model

A two level atom interacting with a quantized electromagnetic field is described by the following Hamiltonian

$$H = \omega_a \sigma_+ \sigma_- + \sum_{\lambda} \omega_{\lambda} a_{\lambda}^{\dagger} a_{\lambda} + \sum_{\lambda} \left(g_{\lambda} \sigma_- \otimes a_{\lambda}^{\dagger} + g_{\lambda}^* \sigma_+ \otimes a_{\lambda} \right), \quad (5.1)$$

where first two terms are the free Hamiltonians of the atom and the field, respectively, the third term is the interaction term, g_{λ} are coupling constants, σ_- , σ_+ are the usual atomic lowering- and raising operators and a_{λ}^{\dagger} , a_{λ} are bosonic creation- and annihilation operators. Total excitation number is a conserved quantity of this model. In the interaction picture with respect to the free Hamiltonians the relevant Hamiltonian that we want to

study is the following

$$H(t) = \sum_{\lambda} \left(g_{\lambda} \sigma_{-} a_{\lambda}^{\dagger} e^{-i(\omega_a - \omega_{\lambda})t} + g_{\lambda}^{*} \sigma_{+} a_{\lambda} e^{i(\omega_a - \omega_{\lambda})t} \right). \quad (5.2)$$

We assume that the system and the environment are initially uncorrelated and that the environment is in the vacuum state. The initial state is thus $|\Psi(0)\rangle = |\varphi\rangle \otimes |0\rangle$. Using the excitation conservation, one can show that the solution to the Schrödinger equation with our initial condition is the following

$$|\Psi(t)\rangle = c_0 |g, 0\rangle + c_1(t) |e, 0\rangle + \sum_{\lambda} c_{\lambda}(t) |0, 1_{\lambda}\rangle. \quad (5.3)$$

The reduced state of the open system is obtained by tracing out the environment degrees of freedom $\rho(t) = \text{tr}_{\text{E}} \{ |\Psi(t)\rangle \langle \Psi(t)| \}$. After relabeling, the solution can be expressed as

$$\rho(t) = \begin{pmatrix} |G(t)|^2 \rho_{ee}(0) & G(t) \rho_{eg}(0) \\ G^{*}(t) \rho_{ge} & \rho_{gg}(0) + (1 - |G(t)|^2) \rho_{ee}(0), \end{pmatrix} \quad (5.4)$$

where the function $G(t)$ is the solution to the following integro-differential equation

$$\begin{aligned} \dot{G}(t) &= - \int_0^t ds f(t-s) G(s), \\ G(0) &= 1. \end{aligned} \quad (5.5)$$

The integrand $f(t-s)$ is related to the environment correlation function $\alpha(t, s) = \text{tr}_{\text{E}} \{ |0\rangle \langle 0| A(t) A^{\dagger}(s) \}$ by $f(t-s) = \alpha(t, s) e^{i\omega_a(t-s)}$ and we have used the following shorthand notation $A(t) = \sum_{\lambda} g_{\lambda} a_{\lambda}^{-i\omega_{\lambda}t}$. In the continuum limit, the integrand can be expressed in terms of the spectral density $J(\omega)$ as

$$f(t-s) = \int d\omega J(\omega) e^{i(\omega_a - \omega)(t-s)}. \quad (5.6)$$

Information about the coupling between the system and the environment is contained in the spectral density.

Whenever $G(t) \neq 0$, an exact time-local master equation for Eq. (5.4) exists

$$\dot{\rho}(t) = - \frac{i}{2} S(t) [\sigma_{+} \sigma_{-}, \rho(t)] + \gamma(t) \left(\sigma_{-} \rho(t) \sigma_{+} - \frac{1}{2} \{ \sigma_{+} \sigma_{-}, \rho \} \right), \quad (5.7)$$

where $\gamma(t)$ is a time dependent decay rate and $S(t)$ is a time-dependent Lamb shift. They are given in terms of $G(t)$ as

$$\begin{aligned}\gamma(t) &= -2\text{Re} \left(\frac{\dot{G}(t)}{G(t)} \right), \\ S(t) &= -2\text{Im} \left(\frac{\dot{G}(t)}{G(t)} \right).\end{aligned}\tag{5.8}$$

The decay rate can be also expressed as $\gamma(t) = -\frac{2}{|G(t)|} \frac{d}{dt} |G(t)|$.

5.1.1 Non-Markovianity of the model

The trace distance measure (3.4) and the measure based on CP-divisibility [22] are compatible for this model. They both signify that the open system dynamics is non-Markovian when $\gamma(t)$ is temporarily negative. It can be shown that the dynamical map for this model is CP-divisible when $|G(t + \tau)| \leq |G(t)|$, for all $\tau > t \geq 0$. Derivative of the trace distance, in Eq. (3.3), takes the following exact form

$$\sigma(\rho, \eta, t) = \frac{2|G(t)|^2 a + |b|^2}{\sqrt{|G(t)|^2 a + |b|^2}} \frac{d}{dt} |G(t)|,\tag{5.9}$$

where $a = \rho_{ee}(0) - \eta_{ee}(0)$ and $b = \rho_{eg}(0) - \eta_{eg}(0)$. In general, if the trace distance between a pair of initial states increases, then the CP-divisibility breaks down. But the CP-divisibility might break down without temporal increase of the trace distance for all pairs of initial states.

5.1.2 Non-Markovian Quantum Jumps

For simplicity we assume that the state of the open system is initially pure. We can express the state of the system for all times as the following convex combination

$$\rho(t) = P[\psi_0, t] |\psi_0(t)\rangle\langle\psi_0(t)| + P[\psi_1, t] |\psi_1\rangle\langle\psi_1|,\tag{5.10}$$

where the states $|\psi_i\rangle\langle\psi_i|$ are normalized and only the state $|\psi_0(t)\rangle$ has explicit time dependence. This decomposition forms the effective ensemble of our unraveling. We have $P[\psi_0, 0] = 1$ corresponding to the initial condition $\rho(0) = |\psi_0(0)\rangle\langle\psi_0(0)|$.

Deterministic evolution is given by the following non-linear equation

$$\begin{aligned} \frac{d}{dt}\psi &= -i\frac{1}{2}\left((S(t) - i\gamma(t))\sigma_+\sigma_- + i\frac{1}{2}\gamma(t)\|\sigma_-\psi\|^2\right)\psi \\ &= \frac{\dot{G}(t)}{G(t)}\sigma_+\sigma_-\psi + \frac{1}{2}\gamma(t)\|\sigma_-\psi\|^2\psi \end{aligned} \quad (5.11)$$

The deterministic evolution of an unnormalized state $\tilde{\psi}$ is given by the linear version of Eq. (5.11). The jump and non-Markovian jump probability densities for this model are

$$P^+[\phi|\psi] = \gamma_+(t)\delta t\|\sigma_-\psi\|^2\delta\left[\phi - \frac{\sigma_-\psi}{\|\sigma_-\psi\|}\right], \quad (5.12)$$

$$P^-[\phi|\psi] = |\gamma_-(t)|\delta t\|\sigma_-\phi\|\frac{P[\phi, t]}{P[\psi, t]}\delta\left[\psi - \frac{\sigma_-\phi}{\|\sigma_-\phi\|}\right]. \quad (5.13)$$

The deterministic evolution rotates superposition states, ground state is invariant with respect to the deterministic evolution, jumps take superposition states into the ground state and non-Markovian jumps create coherent superposition states. This simple analysis confirms that our effective ensemble (5.10) indeed unravels the master equation with the identification $|\psi_1\rangle\langle\psi_1| = |g\rangle\langle g|$. The time evolution of $\psi_0(t)$ can be solved from Eq. (5.11) and it is

$$|\psi_0(t)\rangle = \frac{G(t)c_e(0)|e\rangle + c_g(0)|g\rangle}{\sqrt{|G(t)c_e(0)|^2 + |c_g(0)|^2}}. \quad (5.14)$$

Waiting time distribution

By using the particular expressions for the jump and non-Markovian jump probability densities, we can obtain an expression for the total jump rate $\Gamma[\psi, t] = (\delta t)^{-1} \int d\phi (P^+[\phi|\psi] + P^-[\phi|\psi])$. Since we have only one decay channel, the total jump rate behaves as

$$\Gamma[\psi_0, t] = \begin{cases} (\delta t)^{-1} \int d\phi P^+[\phi|\psi_0] & \text{if } \gamma(t) \geq 0, \\ 0 & \text{if } \gamma(t) < 0, \end{cases} \quad (5.15)$$

$$\Gamma[\psi_1, t] = \begin{cases} 0 & \text{if } \gamma(t) \geq 0, \\ (\delta t)^{-1} \int d\phi P^-[\phi|\psi_1] & \text{if } \gamma(t) < 0 \end{cases} \quad (5.16)$$

Occupation probabilities in the ensemble are $P[\psi_0, t] = \|\tilde{\psi}_0(t)\|^2$ and $P[\psi_1, t] = 1 - \|\tilde{\psi}_0(t)\|^2$. Then from Eq. (4.16) we can solve the waiting

time distribution. For this system, and for other systems where the effective ensemble member ψ_α can act only as a source state for jump or non-Markovian jump over some time interval I there is a simpler way to solve the WTD on I . Since ψ_i , depending on the sign of the decay rate, can act only as a source state for jumps or non-Markovian jumps, the only way that the occupation probability of the state changes is by transitions away from that state. Therefore we have that $P[\psi_i, t + \tau] = P[\psi_i, t] - F[\tau|\psi_i, t]P[\psi_i, t]$, from which we can solve

$$F[\tau|\psi_i, t] = \frac{P[\psi_i, t] - P[\psi_i, t + \tau]}{P[\psi_i, t]}. \quad (5.17)$$

Using the expressions for the occupation probabilities, we can deduce that whenever $\gamma(t) \geq 0$ the waiting time distribution for a jump away from ψ_0 is given by the relative decrease of the norm. Interestingly, when $\gamma(t) < 0$, the waiting time distribution is given by the relative increase of the norm of the deterministically evolving state.

In Fig. 5.1 we have plotted the behavior of the waiting time distribution for this system, when the decay rate takes negative values on some time intervals. Depending on the sign of the decay rate and on the state of the particular realization we see that there are plateaus in the WTD. Those plateaus correspond to the times when the realization cannot jump.

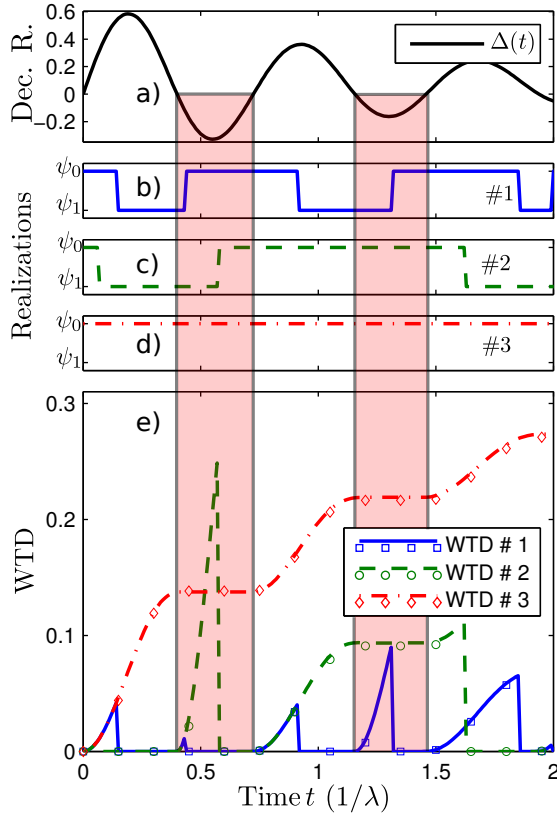


Figure 5.1: Decay rate, three sample realizations of NMQJ process and the waiting time distribution for each realization.

NMQJ from modal dynamics

In order to see how the NMQJ method emerges from the modal dynamics, we choose the preferred property to be the following

$$\pi_{m_N} = \mathbb{I}_S \otimes_\lambda |n_\lambda\rangle\langle n_\lambda| = \mathbb{I}_S \otimes |m_N\rangle\langle m_N|, \quad (5.18)$$

where m_N is a shorthand notation for an arbitrary photon number configuration of the environmental modes. The property states are then

$$|\Psi_{m_N}\rangle = \frac{1}{\sqrt{\mathcal{N}_{m_N}}} |\phi_{m_N}\rangle \otimes |m_N\rangle. \quad (5.19)$$

The modal dynamics between the different property states is given by Eq. (4.17) and the evolution of the property states themselves is determined from the full Schrödinger equation with the Hamiltonian (5.2).

An important observation is that when taking into account the form of the full state in Eq. (5.3), we see that $|\phi_0\rangle\langle\phi_0| = |\psi_0\rangle\langle\psi_0|$ and $|\phi_{1\lambda}\rangle\langle\phi_{1\lambda}| = |\psi_1\rangle\langle\psi_1|$, where ψ_i are the states of the effective ensemble of the NMQJ unraveling. Non-Markovian quantum jumps emerge, when we define new projectors $\Pi_0 = \pi_0$ and $\Pi_1 = \mathbb{I} - \Pi_0$. $\|\Pi_0\Psi(t)\|^2$ and $\|\Pi_1\Psi(t)\|^2$ are the probabilities for the event that the excitation is in the system and for the event that the excitation is in the environment, respectively. In terms of projectors $\Pi_{0,1}$ we define new collective transition rates $\mathcal{T}_{ij}(t)$ and a new collective probability current $\mathcal{J}_{ij}(t)$. We use the term collective because we lose the information in which specific mode of the environment, the excitation is.

When the modal dynamics for the system states is expressed in terms of the collective current, the transition probability (4.20) is equal to the jump probability of the NMQJ method and the transition probability (4.19) is equal to the non-Markovian jump probability of the NMQJ method. This means that the system part of the property states correspond to the two equivalence classes forming the effective ensemble and the transition probabilities between these states are also the same in both methods. The sample paths of these two processes are equal.

For example, we also have the following relation, the collective probability current from the system to the environment, in the continuum limit, is given by $\mathcal{J}_{1,0} = \lim_{N \rightarrow \infty} \sum_{\lambda=1}^N J_{1\lambda,0}(t) = \gamma(t)|G(t)c_e(0)|^2$.

5.1.3 Entanglement trapping

In photonic band gap materials, which are materials where a forbidden region of energies exists in the spectra, Markovian descriptions usually fail because the spectral density is structured. The Hamiltonian (5.2) can be used to study simple models of an atom placed inside some photonic band gap material. An analytically solvable toy model can be constructed by taking the following shape for the spectral density

$$D(\omega) = W_1 \frac{\Gamma_1}{(\omega - \omega_c)^2 + (\Gamma_1/2)} - W_2 \frac{\Gamma_2}{(\omega - \omega_c)^2 + (\Gamma_2/2)}. \quad (5.20)$$

This will result to a gap, i.e. $D(\omega_c) = 0$, if $\Gamma_1 W_2 = \Gamma_2 W_1$. We require that $D(\omega)$ is normalized to 2π , which leads to an additional condition $W_1 - W_2 = 1$. The spectral density itself is defined as $J(\omega) = \rho_\lambda |g_\lambda|^2 = \frac{\Omega_0}{2\pi} D(\omega)$, where $\Omega_0 = \sum_\lambda |g_\lambda|^2$ is the overall coupling. Population trapping occurs when the atom is in resonance with the band gap frequency, i.e. $\omega_a = \omega_c$, and the perfect gap condition is fulfilled.

This model can be solved with the pseudomode method which leads to an interesting structure for the GKSL master equation describing the dynamics of the extended system. The two level atom is coupled to the second pseudomode (PM₂) with coupling Ω_0 , PM₂ is coupled to PM₁ with coupling $V = \sqrt{\Gamma_1\Gamma_2}/2$ and only PM₂ leaks out with a decay rate $\Gamma'_2 = (\Gamma_1 + \Gamma_2)$.

By defining $\eta = \Omega_0/V$, we can express the limiting values for the amplitudes of the atom $c_a(t)$, for the PM₁ $a_1(t)$ and for the vacuum $\Pi_j(t)$ as

$$c_a(\infty) = (1 + \eta^2)^{-1}, \quad (5.21)$$

$$a_1(\infty) = \eta(1 + \eta^2)^{-1}, \quad (5.22)$$

$$\Pi_j(\infty) = \eta^2(1 + \eta^2)^{-1}. \quad (5.23)$$

As one can see, there is significant population trapping in the atom and in the first pseudomode when $\eta < 1$ (weak coupling). PM₂ is empty in this limit, e.g. $a_2(\infty) = 0$.

In the weak coupling ($\eta < 1$), when the trapping occurs, we also observe that the trapped state is an entangled state between the atom and the first pseudomode PM₁, manifested by concurrence.

Interestingly, when the atom has reached a steady state, the reservoir (now in the original picture) is not in a stationary state. This can be evidenced from the reservoir spectrum which shows perpetual oscillations, see Fig. 5.2 a). Thus the population distribution of the modes is ever changing. This effect can be studied also by using the probability currents $J_{\lambda,a}(t)$ (i.e. the probability current from the atom to the mode λ). When the system is in equilibrium, the total current $Q(t) = \int d\omega_\lambda J_{\lambda,a}(t)$ is zero, but the individual components are non-zero, see Fig. 5.2 b). The trapped excitation in the steady state of the atom is coupled to all of the modes and it mediates the observed perpetual redistribution of mode populations.

In the original picture, the atom-mode entanglement and the mode-mode entanglement using the density of entanglement[84] and concurrence is also studied. What we observe is that the atom-mode entanglement and the mode-mode entanglement themselves reach a stationary value (in terms of concurrence) but the entanglement densities themselves do not. See Fig. 5.2 c), d) for the snapshots of the entanglement density between the atom and the modes and between the different modes.

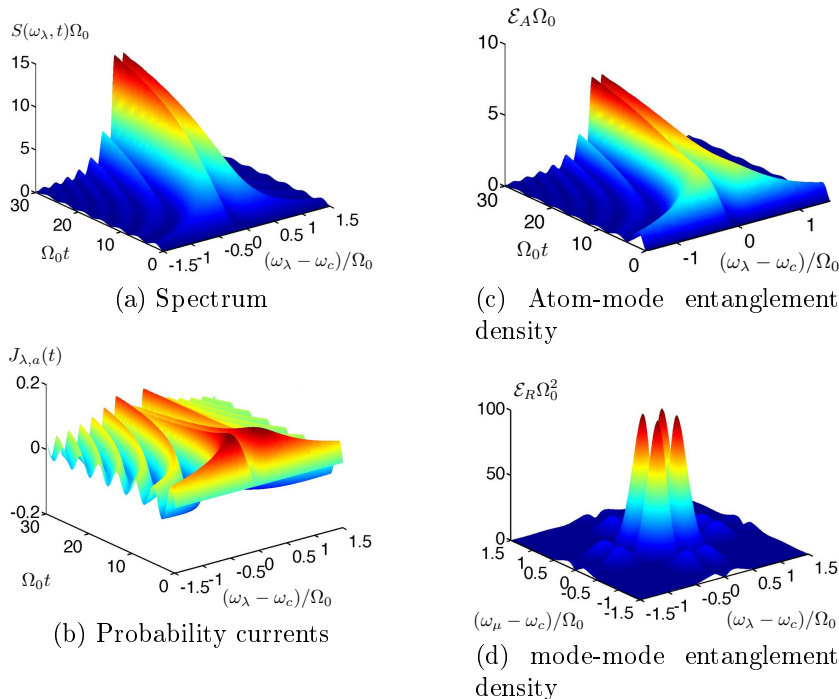


Figure 5.2: In all figures the atom is weakly coupled to the modes and the perfect band gap condition is fulfilled.

5.1.4 Detection of non-Markovianity

By choosing the spectral density as $\rho_\lambda |g_\lambda|^2 = \frac{1}{2\pi} \frac{V^2 \Gamma}{(\omega_\lambda - \omega_c)^2 + (\Gamma/2)^2}$, the Hamiltonian (5.2) is a model for a two level atom inside a lossy cavity. In order to study the non-Markovianity of the model using for example the trace distance criterion, a full state tomography must be made. Using the CP-divisibility criterion for the detection of non-Markovianity, quantum process tomography would be required. For this specific system, we have devised a simpler scheme for the detection of non-Markovianity of the atom dynamics by continuously monitoring the non-memory part of the environment [85].

We assume that initially the atom and the cavity field are in a pure product state in zero temperature. Using the pseudomode method, this system can be mapped into a larger system that obeys the time independent GKSL-equation. The atom is coupled to a pseudomode with a coupling V and the pseudomode, that corresponds to a single cavity mode, leaks to the external environment with a decay rate Γ . Amplitude of the excited state of the atom $c(t)$ and the excited state of the pseudomode $b(t)$ obey

the following system of ordinary differential equations

$$\begin{aligned}\dot{c}(t) &= -iV e^{i\delta t} b(t), \\ \dot{b}(t) &= -\frac{\Gamma}{2} b(t) - iV e^{i\delta t} c(t).\end{aligned}\tag{5.24}$$

The photon flux $R(t)$ emitted from the pseudomode is defined as $R(t) = \Gamma \text{tr} \{ \rho_{AP}(t) a^\dagger a_P \} = \Gamma |b(t)|$. Before the emission, the atom and the pseudomode coherently exchange excitation. After emitting the photon, the atom-pseudomode system is in the ground state $|g, g\rangle$, which is invariant. Therefore, by continuously monitoring the environment of the atom+pseudomode system we do not disturb the non-Markovian dynamics of the atom which arises from the coherent excitation exchange with the pseudomode.

Our measurement signal is $R(t)$. This is maximized if we choose the initial condition to be $|\psi_{AP}(0)\rangle = |e_A, g_P\rangle$, i.e. the atom is initially excited and the pseudomode is empty. With this initial condition, non-monotonic behavior of the excited state population is a signature of the non-Markovian dynamics of the atom. In Fig. 5.3 we emphasize the connection between the non-monotonic behavior of the excited state population of the atom and the photon flux for certain parameter values. As one can see from the figure, the photon flux oscillates almost periodically.

It turns out that when the effect of the damping Γ is negligible, the oscillation of the photon flux is periodic with a frequency

$$\Omega(\delta, V) = \sqrt{4V^2 + \delta^2}.\tag{5.25}$$

By analyzing the signal $R(t)$ more closely, we can identify from the structure of the power spectrum when the dynamics of the atom is non-Markovian. Namely, there is a peak in the vicinity of $\Omega(V, \delta)$ when the dynamics is non-Markovian. Since the photon flux might oscillate also in the parameter region for Markovian dynamics, we must define a threshold frequency Ω_M . In the parameter space (δ, V) , there is a boundary between regions of Markovian and non-Markovian dynamics. Ω_M defines a non-detectability region via $\Omega(V, \delta)$, see Fig. 5.4. If there is peak in the spectrum with $\Omega > \Omega_M$, then the dynamics of the atom is non-Markovian. Structure of the spectrum is illustrated in Fig. 5.5

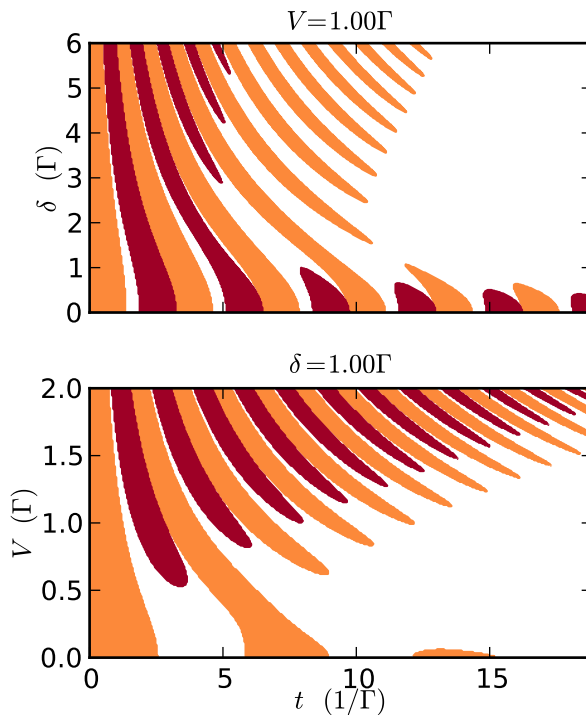


Figure 5.3: **Top:** Regions in the (t, δ) -plane where $C(t) = \partial_t |c(t)|^2 > 0$ (dark red, black) and $B(t) = \partial_t \Gamma |b(t)|^2 > 0$ (orange, gray) for $V = \Gamma$. **Bottom:** Regions in the (t, V) -plane for $\delta = \Gamma$ where $C(t) > 0$ or $B(t) > 0$. Every revival of the atomic population ($C(t) > 0$) is followed by an increase in the photon flux ($B(t) > 0$). There are also areas where $B(t) > 0$ without any previous atomic revivals. For all parameter values the photon flux increases initially.

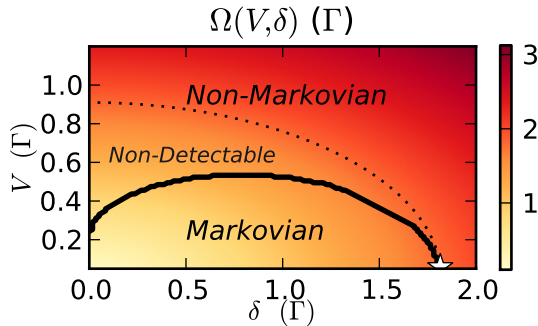


Figure 5.4: Boundary between the Markovian and the non-Markovian dynamical region and the non-detectability region. The maximal Markovian frequency is marked with a white star.

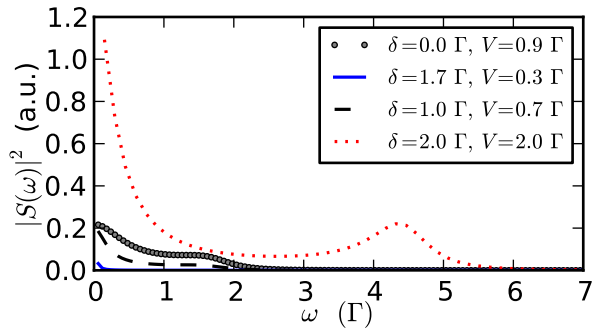


Figure 5.5: Spectrum of the photon flux. $\Omega_M \approx 1.8\Gamma$ is the largest Markovian frequency. In this figure we show evidence that for (δ, V) pair $(2\Gamma, 2\Gamma)$ (dotted red line) non-Markovianity is detected because of a pronounced peak in the flux occurring at $\omega \approx 4.47\Gamma$. Pair $(0.0\Gamma, 0.9\Gamma)$ (dotted gray line) and $(\Gamma, 0.7\Gamma)$ are just below non-detectability border and they show some structure near $\omega \approx \Omega_M$. The solid blue line $(1.7\Gamma, 0.3\Gamma)$ is also near the detectability border and in the Markovian region but there is no significant contribution to the spectrum because the amplitude of $R(t)$ is very small, but there are oscillations.

5.2 Classical non-Markov chain

Equation (2.12) describes the dynamics of an open quantum system. From the time-local master equation for a quantum system it is possible to obtain a description for a classical system by the following construction, for more details see paper **III**.

Assume that $H_{\text{TCL}}(t)$ is time independent and has the following spectral decomposition: $H_{\text{TCL}} = \sum_k E_k |\psi_k\rangle\langle\psi_k|$. Then assume that the system is described by a classical probability distribution, which can be written as $\rho(t) = \sum_k p_k(t) |\psi_k\rangle\langle\psi_k|$, where $p_k(t)$ is the occupation probability of the eigenstate $|\psi_k\rangle$ at time t . Now if $C_k \equiv C_{kl} \equiv |\psi_k\rangle\langle\psi_l|$, a direct calculation from Eq. (2.12) and the fact that $\mathbb{I} = \sum_k |\psi_k\rangle\langle\psi_k|$ gives

$$\dot{p}_k(t) = \sum_{l \neq k} (\gamma_{kl}(t) p_l(t) - \gamma_{lk}(t) p_k(t)), \quad (5.26)$$

which is a classical rate equation. When the rates $\gamma_{kl}(t)$ are positive constants, Eq. (5.26) describes a continuous in time Markov chain. However, if the decay rates turn temporarily negative then this no longer describes a Markov chain but rather a classical non-Markovian process.

Applying Eq. (5.26) to a four site ring configuration (see Fig. 5.6), we get [86]

$$\dot{p}_i(t) = -p_i(t)(\lambda_{i,i+1}(t) + \mu_{i,i-1}(t)) + p_{i-1}\lambda_{i-1,i}(t) + p_{i+1,i}(t)\mu_{i+1,i}(t), \quad (5.27)$$

where $\lambda_{i,i+1}(t)$ is a rate for jumps to the clockwise direction. and the rate for jumps to the anti-clockwise direction is denoted by $\mu_{i-1,i}(t)$. Let us define the following functions

$$r(t) = f(t) - g(t), \quad (5.28)$$

where

$$f(t) = \frac{1}{2}\Gamma (1 + \text{sgn}(\cos(\Gamma\pi t - \pi/2))), \quad (5.29)$$

$$g(t) = \frac{1}{2}\Gamma (1 + \text{sgn}(\cos(\Gamma\pi t + \pi/2))). \quad (5.30)$$

$r(t)$ is a square wave with an amplitude Γ and a period $\frac{2}{\Gamma}$.

System a) in Fig. 5.6 which has only one non-zero rate, $\lambda_{i,i+1}(t) = r(t)$, which may take negative values is a non-Markov chain. The Markovian

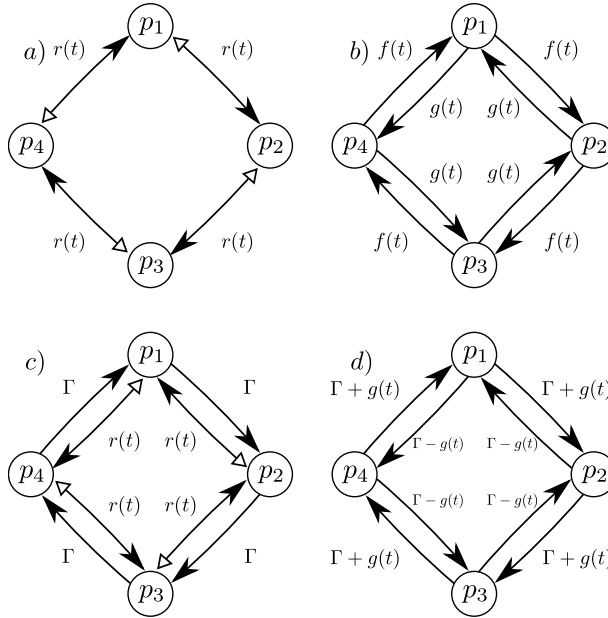


Figure 5.6: The Markov and non-Markov chains considered in the text. The single headed arrows describe a positive rate and the double headed arrows rates oscillating between positive (black head) and negative (white head) values.

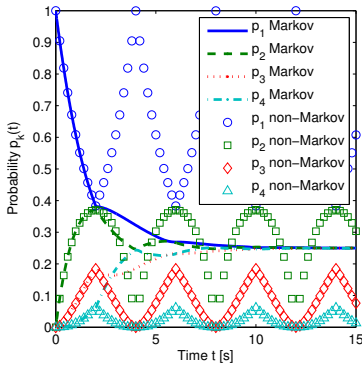


Figure 5.7: Models a) non-Markov and b) Markov from Fig. 5.6, with $\Gamma = \frac{1}{2} 1/s$ and $p_1(0) = 1$.

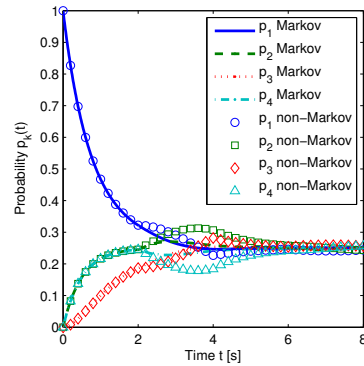


Figure 5.8: Models c) non-Markov and d) Markov from Fig. 5.6, with $\Gamma = \frac{1}{2} 1/s$ and $p_1(0) = 1$.

counterpart for the system a) is the system b) in Fig. 5.6, which has

$\lambda_{i,i+1} = f(t)$ and $\mu_{i,i-1}(t) = g(t)$. In system a) we have a positive rate for jumps to the clockwise direction and a negative rate which corresponds to non-Markovian jumps. In system b) we have positive rates both to the clockwise and anti-clockwise directions. The dynamics of systems a) and b) are plotted in Fig. 5.7. The both systems behave similarly until $r(t)$ changes its sign for the first time, then the non-Markov chain starts to evolve towards its initial state but the Markov chain evolves towards the steady-state.

System c) in Fig. 5.6 is again a non-Markov chain, where is a constant positive rate $\Gamma = \lambda_{i,i+1}$ and an oscillating rate $r(t) = \mu_{i,i-1}(t)$. In this system there is jumps to the clock- and anti-clockwise direction and when $r(t) < 0$ also non-Markovian jumps to the clockwise directions. The Markovian counterpart of the system c) is the system d) in Fig. 5.6. In this system there are the rates $\lambda_{i,i+} = \Gamma + g(t)$ which is equal Γ (when $g(t) = 0$) and 2Γ (when $g(t) = \Gamma$) and $\mu_{i,i-1} = \Gamma - g(t)$ which equals to Γ or 0 depending on the value of $g(t)$. The dynamics of the systems c) and d) are plotted in Fig. 5.8. In this case the non-Markovian effects deviate the time evolution of sites 2 and 4 the most compared to the Markovian evolution. For this configuration of rates, also the non-Markov chain reaches the steady state.

Chapter 6

Quantum discrete dynamics and non-Markovianity

In this section we focus on one dimensional random- and quantum walks. Both the quantum and the random walks, have continuous and discrete in time versions. We focus only on the discrete time versions. The quantum walk is used as a protocol to generate the dynamics that we study. Our main interest is to study the non-Markovianity of the generated discrete dynamics^a.

6.1 Random walks and quantum walks

Canonical example of a random walk is a Markov chain taking values in \mathbb{Z} , where $p(y|x) = \frac{1}{2}\delta_{y,x\pm 1}$, i.e. the walker moves at each step, with certainty, from the current site either one step left or right with equal probability. Let us fix the initial state of the walker to be 0. The probability to reach site $z \in \mathbb{Z}$ after n steps can be obtained using path counting. The number of right or left turns in an n -step path, $0 \rightarrow z$, are $n_- = (n - z)/2$ and $n_+ = (n + z)/2$, respectively. The total number of n -step paths is 2^n . The number of n -step paths, $0 \rightarrow z$, is $K_{0 \rightarrow z}(n) = \binom{n}{n_-} = \binom{n}{n_+} = \frac{n!}{n_+!n_-!}$. Then the probability is simply $P_{n \rightarrow z}(n) = 2^{-n}K_{0 \rightarrow z}(n) = \frac{n!}{2^n n_-! n_+!}$. The standard deviation of the random walk is $\sigma_C(n) = \sqrt{n}$ and the position distribution approaches a Gaussian when n grows.

^aThis chapter contains unpublished material. The experimental implementation of the model to be presented is in progress in Key Laboratory of Quantum Information in USTC, Hefei, China.

When generalizing the above example to the quantum regime, we expect that the state of the walk would be described by a pure state that evolves according to the rules of quantum mechanics, e.g. unitarily. However, there is a no-go theorem [87] that states that in one dimension there cannot exist a non-trivial, homogeneous, local and scalar valued discrete quantum walk. This problem is circumvented by introducing an additional degree of freedom into the the walk, the so called quantum coin. These types of walks are called coined quantum walks. They are described by a unitary transformation W which acts on the elements of $\mathcal{H}_W = \mathcal{H}_C \otimes \mathcal{H}_P = \mathbb{C}^2 \otimes \ell^2(\mathbb{Z})$, where \mathcal{H}_C is the coin space and \mathcal{H}_P is the position space. The unitary transformation W is composed of two parts

$$W = S \cdot (C \otimes \mathbb{I}) = (P_L \otimes T + P_R \otimes T^\dagger) \cdot (C \otimes \mathbb{I}), \quad (6.1)$$

where $P_{L,R}$ are projections onto the left and right pointing basis states $|L\rangle, |R\rangle \in \mathcal{H}_C$, T and T^\dagger act in the following way on the position states $T|z\rangle = |z-1\rangle$, $T^\dagger|z\rangle = |z+1\rangle$ and C is an arbitrary unitary operator acting on \mathcal{H}_C . Evolution of the initial state of the walker $|\Psi_0\rangle$ over n -steps is given by $|\Psi_n\rangle = W^n|\Psi_0\rangle$. It is now obvious, that a quantum walker that is initially localized, can evolve into a superposition state between different positions. Fixing the coin operator to be, for example $C = \frac{1}{\sqrt{2}}(|L\rangle\langle L| + |L\rangle\langle R| + |R\rangle\langle L| - |R\rangle\langle R|)$ (Hadamard coin) one can show that the standard deviation in the position distribution for an asymptotically large n and for a localized initial state, is $\sigma_Q(n) = (1 - \frac{1}{\sqrt{2}})^{\frac{1}{2}}n$ and the position distribution is not Gaussian. Both, the ballistic propagation and the strikingly different position distribution (compared to the classical case) are caused by the interference, see Fig. 6.1.

Natural question to ask is what happens if the interference effects are suppressed. One approach to suppress the coherences is to replace the unitary evolution of the walk $\rho_{n+1} = W\rho_n W^\dagger$ with a quantum channel where errors occur with some probability p

$$\rho_{n+1} = (1-p)W\rho_n W^\dagger + p \sum_j \Omega_j W\rho_n W^\dagger \Omega_j^\dagger \equiv \Lambda(\rho_n), \quad (6.2)$$

where $\sum_j \Omega_j^\dagger \Omega_j = \mathbb{I}$. We have denoted a dynamical map over a single step by Λ . The dynamics of the decoherent walk would be $\rho_n = \Lambda^n(\rho_0)$, where $\Lambda^n = \Lambda \circ \Lambda^{n-1}$, $\Lambda^0 = \mathbb{I}$, $n \geq 1$. For example, the choice $\Omega_j = \mathbb{I} \otimes |i\rangle\langle i|$ corresponds to pure dephasing [88]. In [89] authors choose Ω_j to be a projection to a preferred coin basis, position basis or both (they also study

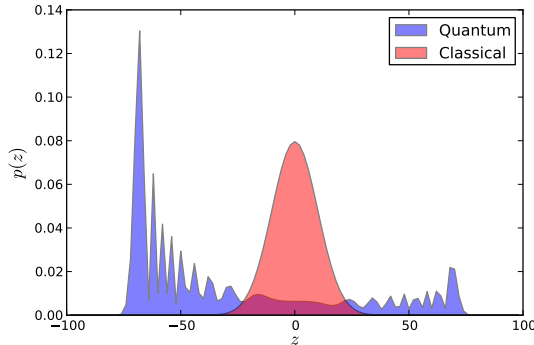


Figure 6.1: Classical walk and quantum Hadamard walk for 100 steps. Quantum walk starts at state $|L, 0\rangle$ and classical walk at site 0.

the effect of imperfect Hadamard operation where the imperfection is controlled by p). They observe that $\sigma_Q(n) \rightarrow \sigma_C(n)$ as $p \rightarrow 1$, i.e. a transition from the quantum (ballistic) to the classical (diffusive) propagation takes place. Another approach to observing the quantum to classical transition, is to extend the coin space and use only parts of it at each step. With this approach the classical limit is reached, when a new coin is used at every time step [90].

One can also use dynamical maps directly to construct quantum walks. One approach is in [91], where open quantum random walks are formulated and their properties are studied. An equivalent formalism to coined quantum walks is the scattering quantum walk (SQW) approach [92, 93]. By using the SQW formalism, classical Markov chains can be systematically quantized [94].

Quantum walks have various applications in quantum information processing. For example, a universal gate set can be constructed using discrete quantum walks [95] and they can be used as a basis for more efficient (than classical) solutions for various search problems [96, 97, 98]. During the recent years, quantum walks have also been implemented experimentally using various techniques, for example using NMR processors [99, 100], trapped atoms [101] and ions [102, 103], photons in waveguide lattices [104], beam splitter arrays [88] and fiber loops [105] have been used. Interesting phenomena such as effects of particle statistics in discrete quantum walk [106] and localization phenomena due to static disorder [107] have been also experimentally observed, to name a few.

6.2 Non-Markovian discrete quantum walk

Engineering a discrete quantum walk that exhibits non-Markovian dynamics requires the protocol generating the dynamics to be generalized from a unitary to a general dynamical map. Using the construction presented in Eq. (6.2) would lead to discrete semigroup dynamics as would also the framework presented in [91].

We use the microscopic approach and construct an explicit model with a specific physical implementation of coined quantum walk in mind, namely a beam splitter array. In this implementation the walker is a single photon. The coin degree of freedom is the polarization of the photon. The position degree of freedom is the spatial location of the photon. In order to make the dynamics of the walker open, we need to couple a subset of the degrees of freedom of the walker to some external environment. Motivated by the recent experiment [108] we couple the coin (polarization) degrees of freedom to the frequency degree of freedom of the photon by using a quartz plate.

The Hilbert space is the following $\mathcal{H} = \mathcal{H}_W \otimes \mathcal{H}_E$. The construction of the unitary operator acting on \mathcal{H} is the following

$$U_{\delta t, i} = \sum_i D_{\delta t, i} \cdot (W \otimes \mathbb{I}_E), \quad (6.3)$$

where W is the usual Hadamard walk operator and $D_{\delta t, i}$ is the unitary operator providing the coupling between the coin- and frequency degrees of freedom. It has the following form

$$D_{\delta t, i} = \int d\omega \sum_{\sigma=L,R} e^{in_{\sigma,i}\omega\delta t_i} |\sigma\rangle\langle\sigma| \otimes |i\rangle\langle i| \otimes |\omega\rangle\langle\omega|, \quad (6.4)$$

where $n_{\sigma,i}$ are polarization and position dependent indices of refraction and δt_i is the interaction time, e.g. the time that the photon spends inside the quartz plate at each step. δt_i is related to the thickness of the quartz plate L_i by $\delta t_i = L_i/c$, where c is the speed of light. This model is schematically presented in Fig. 6.2.

We focus on a homogeneous walk, meaning that $D_{\delta t_i} \rightarrow D_{\delta t}$ and $U_{\delta t, i} \rightarrow U_{\delta t}$. We also assume that the walker always starts from the site 0. If the initial state of the environment is $|\chi\rangle\langle\chi|$, then the dynamical map for n steps is

$$\Phi_n(\rho_0) = \text{tr}_E \left\{ (U_{\delta t})^n (\rho_0 \otimes |\chi\rangle\langle\chi|) (U_{\delta t}^\dagger)^n \right\}, \quad (6.5)$$

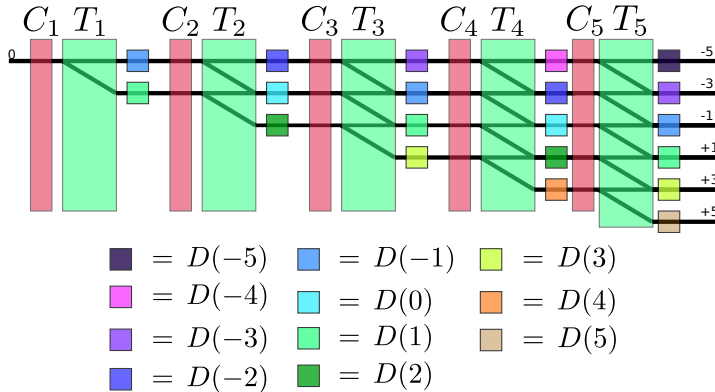


Figure 6.2: Schematic representation of the open quantum walk for five steps. C_i is the i th coin, T_i is the i th shift and $D(z)$ are the position dependent coupling unitaries.

where $\rho_0 = \rho_C \otimes |0\rangle\langle 0|$. Elements of the map can be obtained analytically by using path counting arguments. General element $[\Phi_n]_{m'm,nn';x,y} \equiv \langle m', x | \Phi_n(|m\rangle\langle n| \otimes |0\rangle\langle 0|) |n', y\rangle$ is

$$[\Phi_n]_{m'm,nn';x,y} = \int d\omega |\chi(\omega)|^2 e^{-\frac{1}{2}i\omega\delta t\Delta n(y-x)} \times \langle m', x | (W^n)(|m\rangle\langle n| \otimes |0\rangle\langle 0|) (W^\dagger)^n |n', x\rangle, \quad (6.6)$$

where $|\chi(\omega)|^2 = |\langle \omega | \chi \rangle|^2$ is the frequency distribution of the photon and $\Delta n = n_L - n_R$. The form of the exponential follows from the observation that every path, $0 \rightarrow x$, must contain $n^+(x)$ steps to the right and $n^-(x)$ steps to the left. Similarly for the path $0 \rightarrow y$.

Expression (6.6) consists of two parts; the usual Hadamard walk propagation over n -steps $[W_n]_{m'm,nn';xy} \equiv \langle m', x | (W^n)(|m\rangle\langle n| \otimes |0\rangle\langle 0|) (W^\dagger)^n |n', x\rangle$ and the decoherence function $\gamma(x, y) \equiv \int d\omega |\chi(\omega)|^2 e^{-\frac{1}{2}i\omega\delta t\Delta n(y-x)}$. From this expression we can already deduce some properties of the walk. The position distribution of the walk corresponds to that of a Hadamard walk, since $\gamma(x, x) = 0$. Coupling to the environment modifies the coherences between different sites of the lattice. We demonstrate these effects in Fig. 6.3. The reduced state of the coin is unaffected by the environmental effects.

We will consider only the following class of photon frequency distribu-

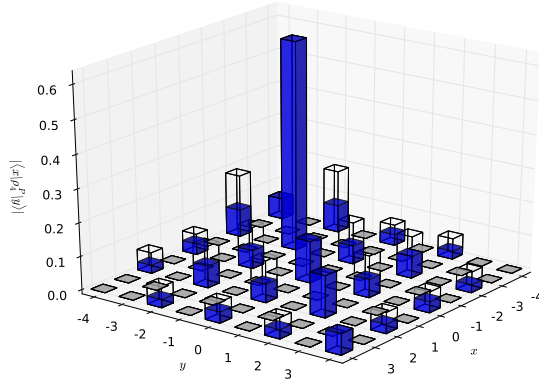


Figure 6.3: Position distribution of the open quantum walk (filled columns) and the Hadamard walk (empty columns) is presented on the diagonal $x = y$. Absolute value of the coherences between different sites $x \neq y$ of the open quantum and the Hadamard walks, are represented by the filled and the empty columns, on the off-diagonal sites. The initial state is $|L\rangle \otimes |0\rangle$ and both walks have been evolved for four steps. The other parameters are $A = 0.5$, $\sigma = 0.18 \cdot 10^{12}\text{Hz}$ and $\delta t \Delta n / \sigma = 13.5$.

tions

$$|\chi(\omega)|^2 = \frac{1}{A} (G(\omega; \mu_1, \sigma) + AG(\omega; \mu_2, \sigma)), \quad (6.7)$$

where $A \in [0, 1]$ and μ, σ are the mean and the standard deviation of Gaussian distribution $G(\omega; \mu, \sigma)$. With this choice, the expression for the decoherence function is

$$\gamma(x, y) = \frac{e^{-\frac{1}{8}\Delta n^2 \delta t^2 \sigma^2 (y-x)^2}}{1+A} \left(e^{\frac{1}{2}i\delta t \Delta n \mu_1 (y-x)} + A e^{\frac{1}{2}i\delta t \Delta n \mu_2 (y-x)} \right), \quad (6.8)$$

$$|\gamma(x, y)| = \frac{e^{-\frac{1}{8}\Delta n^2 \delta t^2 \sigma^2 (y-x)^2}}{1+A} \sqrt{1 + A^2 + 2A \cos\left(\frac{1}{2}\delta t \Delta n \delta \omega (y-x)\right)}, \quad (6.9)$$

where $\delta \omega = \mu_1 - \mu_2$. The coherences between the different positions are exponentially damped as a function of the distance between the sites.

Temporal increase of distinguishability is a sign of non-Markovian dynamics. In the discrete time setting, the temporal change of distinguishability is defined as $\sigma(\rho_1, \rho_2, n) = \frac{1}{2} \|\Phi_{n+1}(\rho_1 - \rho_2) - \Phi_n(\rho_1 - \rho_2)\|_1$, where

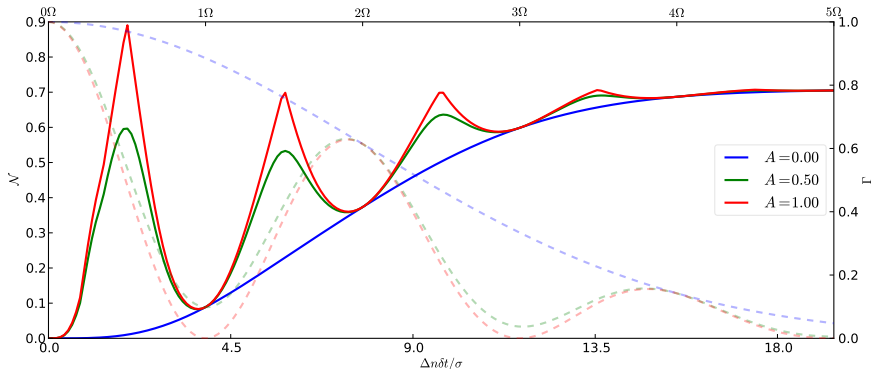


Figure 6.4: The non-Markovianity measure (solid lines, bottom x-scale, left y-scale) and Γ (dashed lines, top x-scale, right y-scale) for three different values of A .

$\mathbb{Z} \ni n \geq 0$. A measure for non-Markovianity is then obtained by accumulating all the increments where the distinguishability has increased. We have plotted the non-Markovianity of the system (solid lines, left y-scale, bottom x-scale) for initial state pair $|L, 0\rangle, |R, 0\rangle$ for 5 steps in Fig. 6.4 as a function of $\Delta n \delta t / \sigma$ (scaled units), for three different values of A and for $\delta \omega = 9\sigma$. From the figure we see that there are points where the structure of the environment does not affect the non-Markovianity of the system. Those points coincide with the solutions of $\cos(\frac{1}{2} \delta t \Delta n \delta \omega) = 1$, e.g. with the periodicity of $\Gamma \equiv |\gamma(x, x+1)|$. We have also plotted Γ (dashed lines, right y-axis, top x-scale) for the same parameter values. Ω is the periodicity of Γ .

Also, if the decoherence is strong enough, then the structure of the environment does not play a role anymore. Here, the critical value is approximately $\delta t \Delta n / \sigma \geq 18.0$. The reason for this is, that irrespectively of the frequency distribution, in the strong decoherence limit, the state of the walker approaches a block diagonal form, e.g. the state is a mixture of localized states. In the strong dephasing regime, the dynamical map can be approximated as

$$\Phi_n(\rho) = \sum_x P_x(W)^n \rho (W^\dagger)^n P_x, \quad (6.10)$$

where $P_x = \mathbb{I} \otimes |x\rangle\langle x|$.

Interestingly, the quantum walk is non-Markovian even when $A = 0$. This should be compared with the experiment reported in [34], where the

choice $A = 0$ resulted in Markovian dynamics. In general, the reason for the non-Markovianity in this case is not the structure of the frequency distribution, although it can enhance the non-Markovianity, but the local unitary operation on the polarization degree of freedom, i.e. the coin flip, which acts as a local control operation [109].

The trace distance evolution for an initial state pair $|L, 0\rangle, |R, 0\rangle$, in the strong dephasing regime is plotted in Fig. 6.5. Initially $\rho_1(0) = |L, 0\rangle\langle L, 0|$

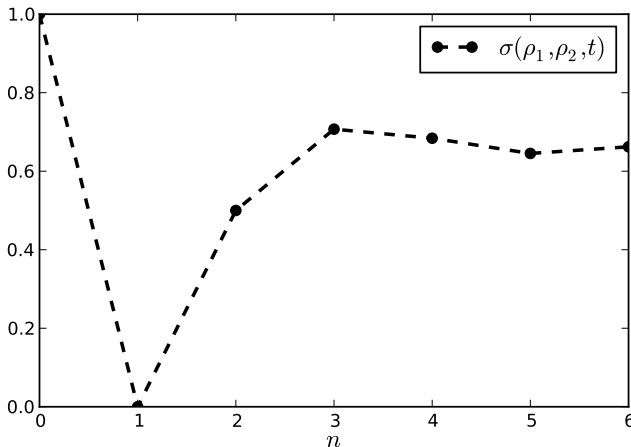


Figure 6.5: The trace distance evolution for the initial state pair $|L, 0\rangle, |0, R\rangle$ for 6 steps. Here $A = 0$, $\delta t \Delta n / \sigma = 18.0$.

and $\rho_2(0) = |R, 0\rangle\langle R, 0|$ are orthogonal. Dephasing is so strong that after the first step the state pair is indistinguishable. Using the map (6.10) we get $\rho_1(1) = \rho_2(1) = \Phi_1(\rho_1(0)) = \Phi_1(\rho_2(0)) = \frac{1}{2}(P_L \otimes P_{-1} + P_R \otimes P_{-1})$. After the second step we get $\rho_1(2) = \frac{1}{4}(P_L \otimes P_{-2} + P_R \otimes P_2 + \sigma_x \otimes P_0)$ and $\rho_2(2) = \frac{1}{4}(P_L \otimes P_{-2} + P_R \otimes P_2 - \sigma_x \otimes P_0)$. The trace distance for this pair is $1/2$, which coincides with the value in Fig. 6.5. This simple calculation demonstrates how the distinguishability might be temporally increased as the coin operation creates coherences that are not destroyed by the dephasing and thus carry information about the initial state.

Chapter 7

Conclusions

In this Thesis we have studied non-Markovian dynamics in general, and especially how classical stochastic processes can be used to generate non-Markovian quantum dynamics.

We have compared the non-Markovian quantum jumps method to a different type of jumplike unraveling that is related to the modal interpretation of quantum mechanics. In paper **I**, We studied the relation between these two approaches using specific models of open quantum systems. The statistical properties of non-Markovian quantum jumps were further analyzed in paper **IV** by constructing the exact waiting time distribution for the stochastic events. We showed how the probabilities for the discontinuous transitions are modified when the dynamics is non-Markovian and discussed some of the problems that arise when the stochastic sample paths are not independent.

The Markovian quantum process is not usually capable to describe correctly the dynamics of an open system that is coupled to a structured reservoir. An example of such system is a model for an atom that is coupled to a band gap. We studied such a model in paper **II** and found an interesting effect of trapped entanglement between the atom and the electromagnetic field. In this work, we also utilized some of the methodology developed in paper **I**

Non-Markovian process is a general concept that exist also classically. There are tools developed for quantum systems that are suitable for studying non-Markovian dynamics but which have not been widely used to study classical systems. In paper **III**, we applied the time convolutionless formalism of quantum master equations to classical systems and allowed the transition rates to take temporarily negative values.

During the recent years, the very definition of quantum non-

Markovianity has been under active research. The different measures of non-Markovianity require a lot of information about the quantum state or the quantum process and this makes the experimental observation of non-Markovian dynamics challenging. In paper **V**, we proposed a simpler approach where the non-Markovianity of the dynamics could be detected by monitoring the temporal behavior of the photon flux emitted from the open system. An experimental implementation of our proposal in a slightly more complicated systems using trapped ions is possible.

Our last topic to study was, the non-Markovianity in discrete dynamical quantum systems. We chose the discrete time quantum walk as our protocol to generate the dynamics. We proposed an experimentally realizable model where non-Markovianity is caused by the local action of the coin. The experimental implementation of the non-Markovian discrete quantum walk by using a beam splitter array is currently under construction.

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