

Quantum Jumps applied to two-level systems.

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1 Introduction

1.1 Closed vs Open

In undergraduate and often times in graduate courses on quantum mechanics, quantum mechanical systems are systematically considered to be closed; that is to say, one assumes that the system in question constitutes all of the information about its evolution, ignoring any interactions that might be present between the system in question and the rest of the universe. This assumption is made tacitly by assuming that Schrödinger's equation governs all quantum phenomena, and that we may always find some Hamiltonian that generates the dynamics. Indeed this is often a great approximation when considering time-independent systems and or highly isolated systems. The Energy spectrum of the Hydrogen atom for example may be deduced via considering this system to be a closed system [1]. Schrödinger's equation is an equation that generates unitary evolution, this will be seen later, as a result there is no dissipation or decoherence [5] which are processes where energy and "quantumness" is not preserved respectively. More on what we mean by "quantumness" in the following section. Decoherence and dissipation are inevitable, every quantum system will experience both of these environmentally induced processes. There do exist interactions which may be approximately described by a closed system with high precision, but in these cases decoherence, a fundamental quantum mechanical process that occurs when a quantum system is measured/interacted with, is explained only by the Copenhagen interpretation [3] of quantum mechanics which says that upon being measured, a quantum system instantaneously collapses to a definite state within the *Hilbert* space associated with the quantum system. This occurs with some probability distribution governing the "collapse", look at the section on POVM [4]. This is at odds with the seemingly continuous world we live in, and one might guess that the Copenhagen school of thought has missed something fundamental. Indeed decoherence is not a phenomenon that occurs instantaneously, decoherence time scales which vary from system to system [11] (pg 66) can actually be computed if one considers the more realistic setting where the system in question, referred to as S in this paper, and the associated environment, referred to as E , are both treated as a quantum system and the system of interest S sits within E , interacting with E via some *Hamiltonian*. A typical "environment" E might be an electromagnetic field which fixes the orientation of a spin amidst the electromagnetic field. If our interest lies in the dynamics of the spin then we may deduce the local dynamics of the spin, now an open system, via partial tracing technique to be discussed in this paper's section 1.4. By considering a larger system one may use our familiar Schrödinger equation as a starting point and later deduce the reduced dynamics of S . Ideally we hope to obtain the unitary evolution for the total dynamics and deduce the dynamics local to S but, as it will be seen in what is to come, this is no easy venture. We will develop methods for deducing the reduced dynamics and apply said methods to a Two-Level system. The resulting equations will be themselves formidably difficult to solve and for this one may turn to Monte-Carlo techniques which is the focus of this paper. The Two-Level system presented is easily soluble via simple ODE methods but will serve as a testing ground for the Quantum Jump approach eluded to here.

1.1.1 Examples of open systems

Quantum mechanics is a theory of matter which is more fundamental than the classical theories afforded by Newtonian dynamics and Maxwell's equations. Quantum mechanics is therefore the correct theory to describe anything around us. In this sense, everything is a Quantum Open system because everything we deemed to be a system will sit within a larger system. If the latter were not to be the case we would inevitably

have to face the Heisenberg-Cut dilemma [15] which asks where does one draw the boundary between the classical and the quantum. Classical beings nevertheless exist in a realm where so called quantum effects may be negligible and classical mechanics is enough to aid us in the understanding of our environment. However, recent interest in technology which is on the Nano scale has functioned as the impetus of a deeper interest regarding the non-unitary (open systems) dynamics of quantum mechanical systems. Some Quantum computers constructed by IBM for example are built from tiny Quantum circuits which are highly susceptible to minuscule disturbances coming from its entourage. In order to truly understand these Quantum circuits and their dynamical properties, a strong understanding of the non unitary evolution must be taken into account and this requires us to consider the quantum system as open. For more information on quantum computers, their hardware components, architecture and interface I recommend the interested reader to visit IBM's webpage [16].

1.2 Unitary Evolution

In the field of Quantum Mechanics for closed systems one is tasked with solving the Schrödinger equation

$$i\partial_t|\psi(t)\rangle = H|\psi(t)\rangle \quad (\hbar = 1) \quad (1)$$

where the state $|\psi(t)\rangle$ is a vector in some *Hilbert* space, call it \mathcal{H}_S , and H is a self-adjoint/Hermitian operator that acts on \mathcal{H}_S . In this paper we may assume that $H \in B(\mathcal{H}_S)$ (the space of bounded linear operators over \mathcal{H}_S since we will be focusing on finite dimensional Quantum Mechanical systems, i.e. systems whose state may be described by a finite dimensional complex valued vector. The notation $|\psi(t)\rangle$ will represent a column vector while the notation $\langle\psi(t)|$ will represent a row vector. Indeed, $|\psi(t)\rangle^\dagger := \langle\psi(t)|$. The solution to equation 1 is

$$e^{-itH}|\psi(0)\rangle \quad (2)$$

where $|\psi(0)\rangle$ is the initial state of the system. However, the story does not end there. We would like to understand the effect of the unitary operator $e^{-itH} := U(t)$ upon acting on $|\psi(0)\rangle$. In general this will require one to solve the eigenvalue problem for the operator H

$$H|\phi_n\rangle = \lambda_n|\phi_n\rangle. \quad (3)$$

Assuming that we have solved the eigenvalue problem for H we may write $|\psi(0)\rangle$ in 2 as follows.

$$U(t)|\psi(0)\rangle = e^{itH} \sum_n \alpha_n |\phi_n\rangle = \sum_n \alpha_n e^{it\lambda_n} |\phi_n\rangle, \quad \{\alpha_k\}_k \in l_2(\mathbb{C}) \quad (4)$$

If the operator H is not too difficult to diagonalize then we have no true hurdles to overcome. In the infinite dimensional case where H is a linear combination of multiplication and differential operators however, things are far from trivial and doing the infinite dimensional analog of diagonalization can present many pitfalls. One highly studied infinite dimensional system is the Quantum Harmonic oscillator with $H = \alpha\hat{p}^2 + b\hat{x}^2$. Diagonalization of such system is successfully done with the *Hermite* functions which are also referred to as the number states in the literature. These types of systems are beyond the scope of this paper but a nice summary of Quantum Harmonic oscillators may be found in [1] chapter 7.

1.3 The Density operator.

Let us take a step back and rewrite the Schrödinger equation as follows [4] (Chapter 2),

$$\rho(t) = -i[H, \rho(t)]. \quad (5)$$

This is called the Liouville-von Neumann (Lv) equation and it is often useful to work with the density operators $\rho(t) := |\psi(t)\rangle\langle\psi(t)|$ rather than vectors. Before we move on let us discuss the operator $\rho(t)$. These so called density operators have the following properties [4](chapter 2). For a pure state, i.e. one of the for $\rho(t) = |\psi(t)\rangle\langle\psi(t)|$

- $\rho(t)$ is a projection operator.
- $\rho(t)^2 = \rho(t)$

- $Tr\{\rho(t)\} = 1 = Tr\{\rho^2(t)\}$.
- $\rho = \rho^\dagger$ (self-adjoint, eigenvalues are real)
- For some observable A , the expectation value is computed as $\langle A \rangle = Tr\{A\rho\}$

Where the trace is defined as follows, letting $\{|\phi_n\rangle\}_n$ be some orthonormal basis spanning the space that $\rho(t)$ is acting on.

$$Tr\{\rho(t)\} = \sum_n \langle \psi_n | \rho(t) | \psi_n \rangle$$

Density operators may be mixtures of a family of density operators as well. We will call these latter types of density operators mixed states. Mixed states will still be positive trace class operators of trace one but their square will no longer be trace 1. i.e. letting $\sigma(t) = \sum_n p_n \rho_n(t)$, with $\sum_n p_n = 1$, it can be shown that $Tr\{\sigma^2(t)\} \leq 1$ [4] (Chapter 2). The aforementioned "quantumness" of a density operator may be quantified by the "purity", defined by $Tr\{\rho^2\}$. If the purity is 1 then we are in the quantum probability regime, while in the case where the purity is 1 we find ourselves in the classical probability regime. To see this let us start with a d dimensional Hilbert space with orthonormal basis $\{|\phi_n\rangle\}_n$ and consider a pure state $\rho(t)$ acting over said space. $\rho(t)$ may then be written as

$$\rho(t) = |\psi(t)\rangle\langle\psi(t)| = \sum_{n,m} \alpha_n(t)\alpha_m^*(t)|\phi_n\rangle\langle\phi_m|. \quad (6)$$

Above we may appreciate the byproduct of the superposition, these are the off-diagonal elements to the state matrix under the representation afforded by the basis $\{|\phi_n\rangle\}_n$ which may be the eigenbasis of some observable of interest. These off-diagonal entries represent the "quantumness" of the relevant system since they are in one-to-one correlation with the superposition of the eigenbasis of a given observable. Via a non unitary process, such as the ones that we will develop in the section to come, the off-diagonal entries banish. Let us now take note of the resulting operator.

$$\rho(t) = |\psi(t)\rangle\langle\psi(t)| = \sum_n |\alpha_n(t)|^2 |\phi_n\rangle\langle\phi_n| \quad (7)$$

If we consider a time independent uniform distribution for the $|\alpha_n(t)|^2$, then the sate above is simply

$$\rho(t) = |\psi(t)\rangle\langle\psi(t)| = \sum_n \frac{1}{d} |\phi_n\rangle\langle\phi_n| \quad (8)$$

where, again, d is the dimension of the space spanned by $\{|\phi_n\rangle\}$. The trace of 8 is easily computed to be $\frac{1}{d}$. 8 is classical because it associates a classical probability distribution to the observable whose eigenvectors are $\{|\phi_n\rangle\}$.

Let us now return to 5, solving Lv it immediately follows that

$$\rho(t) = U(t)\rho(0)U^\dagger(t) := \mathcal{U}_t(\rho(0)) \quad (9)$$

i.e. the time evolution of some initial density operator $\rho(0)$ is generated by a unitary map \mathcal{U}_t . In general the closed system approximation does not hold and one must allow for non-unitarity when treating a Quantum Mechanical system. i.e. the evolution of some initial state matrix $\rho(0)$ would instead be governed by some unitary map \mathcal{U}_t that is an automorphism from the space of trace one trace class operators that are self adjoint onto itself. In such cases equation would have to be replaced with something involving a completely positive map Λ_t [6] forming part of a so called Quantum dynamical semigroup which we will define shortly under the name of dynamical maps below. However, to understand what is to come we must first develop further the trace map and introduce the notion of partial trace.

1.4 Partial trace

The point of departure for quantum open systems is assuming that the system in question is interacting with another systems which we will call the environment. The total dynamics will not be what we will be interested in but rather the local dynamics of the system of interest. To treat compound quantum systems one

need only construct bigger *Hilbert* spaces. If we have a quantum system whose state $|\psi_S\rangle$ evolves within the space \mathcal{H}_S and interacts with another quantum system whose state $|\psi_E\rangle$ evolves within the *Hilbert* space \mathcal{H}_E then the the total state of the compound system to be in the space $\mathcal{H}_S \otimes \mathcal{H}_E$. The most general state that describes the state of the compound quantum system in question will be of the form

$$\sum_{i=1}^{\min\{n,m\}} \alpha_i |\psi_i\rangle \otimes |\phi_i\rangle \quad (10)$$

where $\{|\psi_i\rangle\}_{i=1}^m$ and $\{|\phi_i\rangle\}_{i=1}^n$ are orthonormal basis (ONB) for H_S and H_E respectively. This is called a *Schmidt* decomposition [4].

1.4.1 The environment as a quantum system

Let us take the environment to be the system, also quantum, whose state evolves in the *Hilbert* space \mathcal{H}_E , $\dim(\mathcal{H}_E) = n$ with ONB $\{E_i\}_i$. The "system" S will be a quantum system whose state lives in the *Hilbert* space \mathcal{H}_S , $\dim(\mathcal{H}_S) = m$ with ONB $\{|\psi_i\rangle\}_i$. The total state of the compound system will therefore live in $\mathcal{H}_S \otimes \mathcal{H}_E$. Compound quantum systems of this form are the building blocks of a quantum open systems if the dynamics is generated by a *Hamiltonian* $H_{SE} = H_S + H_E + H_I$ which includes the interaction dynamics between the system and the environment H_I . Ignoring the dynamics for now let $|\psi_{SE}(0)\rangle$ be some initial state, then in general it will have the form

$$|\psi_{SE}(0)\rangle = \sum_{i=1}^m \alpha_i |\psi_i\rangle \otimes |E_i\rangle. \quad (11)$$

The corresponding density matrix is

$$|\psi_{SE}(0)\rangle\langle\psi_{SE}(0)| = \rho_{SE} = \sum_i \sum_j \alpha_i \alpha_j^* |\psi_i\rangle\langle\psi_j| \otimes |E_i\rangle\langle E_j|. \quad (12)$$

Here we have the state of the total system. However, if we are only interested in how S evolves with time, or what the local state of the system S is, we need a way to deduced the local dynamics. How do we obtain the state matrix pertaining only to the system S ? It turns out that we need to trace out the degrees of freedom pertaining to the environment [5](Chapter 2). The resulting matrix, $Tr_E\{\rho_{SE}(0)\}$, is the state matrix of the system S , call it ρ_S . The partial trace Tr_E is defined as follows.

Definition 1. $Tr_E\{\cdot\} : T(\mathcal{H}_S \otimes \mathcal{H}_E) \rightarrow T(\mathcal{H}_S)$ The partial trace Tr_E is a mapping from the density matrices $\rho_{SE} = |\psi_{SE}\rangle\langle\psi_{SE}|$ in the Banach space $T(\mathcal{H}_S \otimes \mathcal{H}_E)$ of trace-class operators on the Hilbert space $\mathcal{H}_S \otimes \mathcal{H}_E$ to $\rho_S \in T(\mathcal{H}_S)$.

$$Tr_E\{|\psi_{SE}\rangle\langle\psi_{SE}|\} := \sum_i \langle\phi_i|\psi_{SE}\rangle\langle\psi_{SE}|\phi_i\rangle$$

$\{|\phi_i\rangle\}$ is some ONM of \mathcal{H}_E , it can be shown that the partial trace is basis independent.

This mapping yields the appropriate reduced dynamics that allows us to see how the environment E affects our system S without having to keep track of what the environment is doing. Here is the partial trace of the state in equation 12.

$$\begin{aligned} Tr_E\{\rho_{SE}(0)\} &= \sum_k \sum_i \sum_j \alpha_i \alpha_j^* |\psi_i\rangle\langle\psi_j| \langle E_k|E_i\rangle\langle E_j|E_k\rangle = \\ &= \sum_i \sum_k \alpha_i \alpha_k^* |\psi_i\rangle\langle\psi_k| \langle E_k|E_i\rangle = \\ &= \sum_k |\alpha_k|^2 |\psi_k\rangle\langle\psi_k|. \end{aligned} \quad (13)$$

This is an astonishing results for two reasons. First, the resulting matrix is diagonal. Taking the partial trace over the perfectly distinguishable environmental degrees of freedom has induced optimal decoherence (i.e.

all of the off-diagonal elements are zero). Second, the resulting density matrix is a "mixed" state. This is critical because the total state matrix prior to the partial tracing was a "pure" state. With this "reduced" density matrix we can compute expectation values of any local observable, A_S (self-adjoint) over \mathcal{H}_S as follows

$$\langle A_S \rangle = Tr_S\{\rho_S A_S\}. \quad (14)$$

To reassure ourselves that the partial trace Tr_E is the appropriate mapping to use in order to deduce the local dynamics lets consider an arbitrary observable A_S over \mathcal{H}_S , there is a natural embedding of such an observable that extends it to the space of observables over $\mathcal{H}_S \otimes \mathcal{H}_E$.

$$A_S \rightarrow A_S \otimes I_E,$$

where I_E is the identity matrix in the \mathcal{H}_E . In quantum open systems one primarily interest themselves in the statistical properties pertaining to observables of the form $A_S \otimes I_E$. One can obtain the expectation value of such an observable by using the total system's state matrix as follows

$$\langle A_S \otimes I_E \rangle = Tr\{\rho_{SE}(A_S \otimes I_E)\}.$$

But for the separable case $\rho_{SE} = \rho_S \otimes \rho_E$ one immediately sees that

$$Tr\{\rho_{SE}(A_S \otimes I_E)\} = Tr\{\rho_S A_S \otimes \rho_E\} = Tr_S\{\rho_S A_S\} Tr_E\{\rho_E\} = Tr_S\{\rho_S A_S\}.$$

This means that precisely all of the information need to compute the statistical properties of some observable in the system S is contained in the reduced density matrix ρ_S .

1.4.2 Environmentally induced non-unitarity

Let H_{SE} be the *Hamiltonian* governing the dynamics of some quantum open system. Assuming that the *Hamiltonian* is time independent, we can immediately make form of the time evolution operator of the compound system. i.e. $U = e^{-itH_{SE}}$. Assuming that the system and the environment are uncorrelated at $t = 0$, i.e. $\rho_{SE}(0) = \rho_S(0) \otimes \rho_E(0)$ and evolving the state matrix using the time evolution operator as well as tracing out the environmental degrees of freedom we arrive at the following

$$\rho_S(t) = Tr_E\{U(t)(\rho_S(0) \otimes \rho_E(0))U^\dagger(t)\}. \quad (15)$$

Now, assuming that the environment is in the state $\rho_E(0) = \sum_i p_i |E_i\rangle\langle E_i|$ at $t = 0$ (this is immaterial and does not affect generality) the above reduces to

$$\rho_S(t) = \sum_{ij} p_i \langle E_j | U(t) | E_i \rangle \rho_S(0) \langle E_i | U^\dagger(t) | E_j \rangle. \quad (16)$$

The operators $\langle E_j | U(t) | E_i \rangle$ are called Kraus operators [2] and these operators evolve the state of the system S non-unitarily. The Kraus operators carry information about the environments initial state and the dynamics of the joint system SE , furthermore the map $\Lambda_t := \sum_{ij} p_i \langle E_j | U(t) | E_i \rangle [\dots] \langle E_i | U^\dagger(t) | E_j \rangle$ is a trace preserving completely positive map and these Kraus operators have the property $\sum_{ij} \langle E_j | U(t) | E_i \rangle \langle E_i | U^\dagger(t) | E_j \rangle = I_S$. The non-unitarity can present itself explicitly in two ways.

- The first is decoherence. The decaying of the off-diagonal elements in the reduced state matrix $\rho_S(t)$. Quantum coherences (i.e. interference terms, off-diagonal terms) are very delicate and if there is an environment interacting with our system then the system is essentially being "measured" continuously by said environment and measurements eliminate quantum coherences. We deliberately use the term *measurement* in order to connect this description of decoherence to that of the Compenhagen interpretation. This is a side note and we will have very little else to say about decoherence in this paper. The interested reader may turn to the paper "Decoherence" by Schlosshauer [5]
- The second is dissipation, it is a common mistake to consider dissipation and decoherence as analogous or even synonymous but this is incorrect. Indeed one can have decoherence without dissipation even though dissipation is always accompanied by decoherence. A model that exhibits decoherence but no dissipation is recoil less scattering for example. This is a very interesting model because although the particles self dynamics are taken to be that of a free particle unhindered by the environmental scattering, the system nevertheless undergoes exponential decoherence in in the position basis due to the interaction with the environment.

The problem is now evident, 16 requires us to compute the inner products $\langle E_j|U(t)|E_i\rangle$ but this is in general an intractable task for many quantum open systems due to the requirement that we solve the eigenvalue problem for the H_{SE} . In practice it is the interaction terms in H_{SE} that are quite challenging to work with. Even if the eigen value problem for H_E and H_S is solved, both operators acting on different subspaces of $\mathcal{H}_S \otimes \mathcal{H}_E$, the inclusion of H_I forces the requirement of diagonalizing an operator acting on the total space $\mathcal{H}_S \otimes \mathcal{H}_E$ which is a formidable task.

In the case where we would like to avoid the eigenvalue problem for H_{SE} we may work with the differential version of 16. Before further discussing the differential version of 16 let us return to the maps $\Lambda(t)$ and motivate them a bit more. Let us assume that $\rho_{SE}(0) = \rho_S(0) \otimes \rho_E(0)$. From 16 we have

$$\rho_S(t) = \sum_{ij} p_i \langle E_j|U(t)|E_i\rangle \rho_S(0) \langle E_i|U^\dagger(t)|E_j\rangle. \quad (17)$$

A mapping defined as above,

$$\Lambda_t \rho_S(0) := \sum_{ij} p_i \langle E_j|U(t)|E_i\rangle \rho_S(0) \langle E_i|U^\dagger(t)|E_j\rangle. \quad (18)$$

is an instance of a *dynamical map* [10].

Definition 2. *Dynamical map (informal definition):* $\Lambda_t : \rho(0) \rightarrow \rho(t)$ is said to be a dynamical map if it takes an arbitrary quantum state $\rho(0)$ to a final quantum state $\rho(t)$ at some fixed t in accordance with the rules of quantum mechanics.

Recall that 18 is obtained simply via the unitary evolution of the compound system and a partial trace over environmental degrees of freedom. Schrödinger's equation is responsible for the dynamics and therefore 18 is in accord with the rules of quantum mechanics making it a dynamical map. The Kraus operators [2] $\langle E_j|U(t)|E_i\rangle$ now written as $W_{ji}(t)$ are trace preserving operators over the *Banach* space of statistical operators, i.e. trace class operators with trace one, satisfying the completeness constraint

$$\sum_{ij} W_{ij}(t) W_{ji}^\dagger(t) = I_S. \quad (19)$$

The number of Kraus operators required to represent a dynamical map will always be bounded by $\dim(\mathcal{H}_S)^2$. The most general way an open quantum system may evolve is expressed by 16, therefore any dynamical map can be completely characterized in terms of a set of Kraus operators $\{W_{ij}\}_{ij}$. The classification problem for completely positive maps has been solved and the relevant result is known as Choi's theorem. This description given for dynamical maps is very informal and will be the one used in the remainder of this paper, a more formal definition is provided but not elaborated upon. In what follows $\mathcal{D}(\mathcal{H}_S)$ is the space of statistical operators, i.e. density matrices of the system S .

Definition 3. *Dynamical map (formal)* A map $\Lambda_t := \mathcal{D}(\mathcal{H}_S) \rightarrow \mathcal{D}(\mathcal{H}_S)$ is a dynamical map iff it is a completely positive map, has convex linearity and is trace preserving.

The family of dynamical maps $\{\Lambda_t | t \geq 0\}$ satisfying the semigroup condition $\Lambda_s \Lambda_t = \Lambda_{s+t}$ forms what is referred to as a *quantum dynamical semigroup*. It can be shown that, under certain assumptions (we will return to what these assumptions are later), there exists an operator \mathcal{L} , as illustrated in Alicki et al [9] such that

$$\Lambda_t = e^{\mathcal{L}t}. \quad (20)$$

Now let us differentiate, a special type of derivative is needed here but we will not go into it, in the end it all works out and the calculation below makes sense.

$$\frac{\partial}{\partial t} \rho_S(t) = \frac{\partial}{\partial t} \nu_t \rho_S(0) = \frac{\partial}{\partial t} e^{\mathcal{L}t} \rho_S(0) = \mathcal{L} \nu_t \rho_S(0) = \mathcal{L} \rho_S(t). \quad (21)$$

\mathcal{L} is called the *Lindbladian* [11], we can therefore conclude that the *Lindbladian* is the generator of the dynamical semigroup $\{\Lambda_t | t \geq 0\}$. This yields a so called master equation. For a general finite dimensional Hilbert space $\mathcal{H}_S = N$, $\dim \mathcal{H}_S$, the most general form of \mathcal{L} is

$$\mathcal{L} \rho_S(t) = -i[H_S, \rho_S(t)] + \frac{1}{2} \sum_{n=1}^{N^2} \{2C_n \rho_S(t) C_n^\dagger - C_n^\dagger C_n \rho_S(t) - \rho_S(t) C_n^\dagger C_n\}. \quad (22)$$

This is known as the GKSL (Gorini–Kossakowski–Sudarshan–Lindblad) equation and more may be learned about it in [17]. The operators C_n are a set of N^2 linear operators forming an orthonormal basis for the space $\mathcal{B}(\mathcal{H}_S)$ [9], one of these elements will be proportional to the identity. The difficulty now lies in solving the equation

$$\partial_t \rho_S(t) = -i[H_S, \rho_S(t)] + \frac{1}{2} \sum_{n=1}^{N^2} \{2C_n \rho_S(t) C_n^\dagger - C_n^\dagger C_n \rho_S(t) - \rho_S(t) C_n^\dagger C_n\}$$

which is equivalent to 22. In practice one arrives to such an equation via first considering the total Lv equation

$$\rho_{SE}(t) = -i[H_{SE}, \rho_{SE}(t)] \quad (23)$$

partial tracing over the environmental degrees of freedom. Under the so called Born-Markov approximation such a partial trace leads to the GKSL equation.

2 Master Equations

So far we have tackled open systems by first computing the total system plus environment dynamics, unitary time evolution $U(t)$, and tracing out the environmental degrees of freedom after evolving some initial compound state $\rho_{SE}(0)$. Although the evolution due to U is unitary, tracing over the environmental degrees of freedom will in general yield non-unitary dynamics. Unfortunately this approach requires that we solve the eigenvalue problem in order to compute the inner products in equation 16. An approach more suited to the Markov-Born limiting case [8] which we will formalize in this section allows us to instead start with the relevant Lv equation.

$$\partial_t \rho_{SE}(t) = -i[H_{SE}, \rho_{SE}(t)] \quad (24)$$

and solve by first taking the partial trace over the environment which yields a differential equation for the evolution of the reduced density matrix.

$$\partial_t \rho_S(t) = -i \text{Tr}_E \{ [H_{SE}, \rho_{SE}(t)] \} \quad (25)$$

The partial trace term leads to a non-unitary dynamics which takes the form of a formidable differential equation which solutions are in general intractable, both analytically and numerically, for any practical case. Fortunately one is usually not interested in the dynamics of the environment, this allows us to focus only on the system and the interaction dynamics. The mathematical treatment of the environment in this case may be of some bath whose dynamics are approximately unperturbed by the system, this type of approximation is referred as the *Born* approximation [8] (Chapter 3). This defines a specific type of open quantum system whose initial and evolved states take the form $\rho_{SE}(0) = \rho_S(0) \otimes \rho_E(0)$ and $\rho_{SE}(t) = \rho_S(t) \otimes \rho_E(0)$ respectively. Now, using this assumption the reduced (Lv) is approximately

$$\partial_t \rho_S(t) = -\frac{i}{\hbar} \text{Tr}_E \{ [H_{SE}, \rho_S(t) \otimes \rho_E(0)] \}, \quad (26)$$

formally integrating this equation we arrive at

$$\rho_S(t) = \rho_S(0) - i \int_0^t dt_1 \text{Tr}_E [H_{SE}, \rho_S(t_1) \otimes \rho_E(0)]. \quad (27)$$

Let us now substitute equation 27 into 26.

$$\partial_t \rho_S(t) = -i \text{Tr}_E \{ [H_{SE}, \rho_S(0) \otimes \rho_E(0)] \} + \frac{i^2}{\hbar^2} \int_0^t dt_1 \text{Tr}_E \{ [H_{SE}, [H_{SE}, \rho_S(t_1) \otimes \rho_E(0)]] \} \quad (28)$$

This equation will be referred to as the *pre-Markovian* equation. We could formally integrate the above and substitute the result back into 28 to obtain a term of third order in t , repeating this process indefinitely yields a convoluted iterative solution to the dynamics. We will not bother expanding the series completely and will stop at 28 and use such an equation to derive the so called *Born–Markov Master* equation (BMME) which is a local in time version of 28 obtained from appropriate approximations. In a nutshell the BMME amounts to replacing the t_1 in the state $\rho_S(t_1) \otimes \rho_E(0)$ with a t in 28. One then is left with the task of computing the

resulting integral. There will be time dependence afforded by the H_{SE} because here the interactive frame is being used and H_{SE} is actually $e^{-it(H_S+H_E)}H_{SE}e^{it(H_S+H_E)}$. We swept the latter detail under the rug as to not make this paper lengthier than it has already become. An at length discussion of the above may be found in [8]. We present the Born-Markov approximation [8] assumptions below and then present an example.

1. Separability: At $t = 0$ there are no correlations between the system and its environment such that the total density matrix can be written as a tensor product $\rho_{tot}(0) = \rho_{sys}(0) \otimes \rho_{env}(0)$.
2. Born approximation: Requires: (1) that the state of the environment does not significantly change as a result of the interaction with the system; (2) The system and the environment remain separable throughout the evolution. These assumptions are justified if the interaction is weak, and if the environment is much larger than the system. In summary, $\rho_{tot}(t) \approx \rho_{sys}(t) \otimes \rho_{env}(0)$.
3. The time-scale of decay for the environment τ_{env} is much shorter than the smallest time-scale of the system dynamics $\tau_{sys} \gg \tau_{env}$. This approximation is often deemed a ‘‘short-memory environment’’ as it requires that environmental correlation functions decay on a time-scale fast compared to those of the system
4. Secular approximation: Stipulates that elements in the master equation corresponding to transition frequencies satisfy $|\omega_{ab} - \omega_{cd}| \ll \frac{1}{\tau_{sys}}$, i.e., all fast rotating terms in the interaction picture can be neglected. It also ignores terms that lead to a small renormalization of the system energy levels. This approximation is not strictly necessary for all master-equation formalisms (e.g., the Block-Redfield master equation [8](Chapter 3)), but it is required for arriving at the Lindblad form 22.

2.1 Spontaneous emission

We further develop the theory of non-unitary dynamics and decoherence, in particular those governed by a BMME via an example. Consider a two-level atom coupled to a bath and let the *Hamiltonian*

$$H_{SE} = \frac{\omega_a}{2}\sigma_z + \sum_k \omega_k b_k^\dagger b_k + \sum_k (g_k b_k + g_k b_k^\dagger)(\sigma_+ + \sigma_-) \quad (29)$$

describe the dynamics of the total system. Here we use the convention $A \otimes B := AB$ for the sake of visual clarity. $H_S = \frac{\hbar\omega_a}{2}\sigma_z$ is the self *Hamiltonian* of the system, $H_I = \sum_k (g_k^* b_k + g_k b_k^\dagger)(\sigma_+ + \sigma_-)$ is the interaction *Hamiltonian* and $H_E = \hbar \sum_k \omega_k b_k^\dagger b_k$ is the bath *Hamiltonian* of the environment. We will not elaborate in the spin algebra for the two level system nor the ladder operators of the quantum harmonic oscillator being used here but any introductory quantum text book [1] will suffice as a resource to study this operators as well as motivate them. Before moving on, we will switch to the interaction picture in order to simplify things a bit. This allows us to trade in the equation

$$\partial_t \rho_{SE}(t) = -\frac{i}{\hbar} [H_{SE}, \rho_{SE}(t)] \quad (30)$$

for the equivalent

$$\partial_t \rho_{int}(t) = -\frac{i}{\hbar} [H_{int}, \rho_{int}(t)]. \quad (31)$$

The new figures are defined bellow.

- $\rho_{int}(t) = e^{it(H_S+H_E)} \rho_{SE}(t) e^{-i(H_S+H_E)}$
- $H_{int} = e^{it(H_S+H_E)} H_I e^{-it(H_S+H_E)}$

The operator H_{int} simplifies to

$$\hbar \sum_k g_k (b_k^\dagger \sigma_+ e^{it(\omega_a+\omega_k)} + b_k \sigma_+ e^{it(\omega_a-\omega_k)} + b_k \sigma_- e^{-it(\omega_a+\omega_k)} + b_k^\dagger \sigma_- e^{-it(\omega_a-\omega_k)})$$

with some help from the Baker-Campbell-Hausdorff theorem, wikipedia has a great over view on this theorem if interested, I am using a lemma/ special case of this theorem.

$$e^X Y e^{-X} = Y + [X, Y] + \frac{1}{2!} [X[X, Y]] + \frac{1}{3!} [X, [X, [X, Y]]] + \dots$$

In systems of this sort it is often reasonable to remove the terms involving $\omega_a + \omega_k$ in the argument and retain only the terms involving $\omega_a - \omega_k$. $\omega_a + \omega_k$ is expected to be much larger than $\omega_a - \omega_k$, more can be said about this but it would go beyond the scope of this paper so we refer the interested reader to the excellent paper on the subject by Fuji [7] or Townsend's text [1]. This type of approximation is known as the *Rotating Wave Approximation* and it merits use on the grounds that the terms involving $\omega_a + \omega_k$ in the argument simply average to zero in the time frame we are interested in and can thus be ignored without a significant contribution to error.

$$H_{int} \approx \sum_k g_k (b_k \sigma_+ e^{it(\omega_a - \omega_k)} + b_k^\dagger \sigma_- e^{-it(\omega_a - \omega_k)}). \quad (32)$$

We may now take our approximated H_{int} and plug it into equation 28 assuming that the *Born* approximation is also applicable, indeed it is since a sea of oscillators can hardly be influenced by a single two-level atom. Our pre-*Markovian* equation in this case is

$$\begin{aligned} \partial_t \rho_S(t) = & -\frac{i}{\hbar} Tr_E \left\{ \left[\hbar \sum_k (a_k(t) b_k \sigma_+ + a_k^*(t) b_k^\dagger \sigma_-), \rho_S(0) \otimes \rho_E(0) \right] \right\} \\ & + \frac{i^2}{\hbar^2} \int_0^t dt_1 Tr_E \left\{ \left[\hbar \sum_k (a_k(t) b_k \sigma_+ + a_k^*(t) b_k^\dagger \sigma_-), \left[\hbar \sum_{k'} (a_{k'}(t_1) b_{k'} \sigma_+ + a_{k'}^*(t_1) b_{k'}^\dagger \sigma_-), \rho_S(t_1) \otimes \rho_E(0) \right] \right] \right\}. \end{aligned} \quad (33)$$

$\rho_S(t)$ is actually $\rho_{S_{int}}(t)$ but we remove the second subscript for clarity and a_k is defined as $g_k e^{it(\omega_a - \omega_k)}$. To move forward an initial state must be specified, let $\rho_{SE}(0) = \rho_S(0) \otimes |\Omega\rangle_E \langle \Omega|$. The system's initial state is yet to be defined and the environment is in the vacuum state, i.e. ground state. We can compute $Tr_E \{ [\sum_k (a_k(t) b_k \sigma_+ + a_k^*(t) b_k^\dagger \sigma_-), \rho_S(0) \otimes |\Omega\rangle_E \langle \Omega|] \}$ with relative ease. Using linearity of the commutator and some properties of the tensor product, note that we have been using the short hand $b_k \sigma_+$ when referring to $b_k \otimes \sigma_+$, we can rewrite the above commutator as follows.

$$\sum_k [\sigma_+ + \sigma_-, \rho_S(0)] Tr_E \{ [a_k b_k + G_k^* b_k^\dagger, |\Omega\rangle_E \langle \Omega|] \}. \quad (34)$$

But $Tr_E \{ [a_k b_k + a_k^* b_k^\dagger, |\Omega\rangle_E \langle \Omega|] \} = \sum_i \langle E_i | ([a_k b_k + a_k^* b_k^\dagger, |\Omega\rangle_E \langle \Omega|]) | E_i \rangle$. The only term in the trace that is non zero is the summand originating from the vacuum element. The trace therefore simplifies to

$$\langle \Omega | a_k b_k | \Omega \rangle - \langle \Omega | a_k b_k | \Omega \rangle + \langle \Omega | a_k^* b_k^\dagger | \Omega \rangle - \langle \Omega | a_k^* b_k^\dagger | \Omega \rangle,$$

which is zero since $b|\Omega\rangle = 0$ and $\langle \Omega | b^\dagger = 0$. Furthermore it can be shown that the integral term in equation (60) can be reduced to

$$\int_0^t dt_1 \sum_k Tr_E \{ [(a_k(t) b_k \sigma_+ + a_k^*(t) b_k^\dagger \sigma_-), [a_k(t_1) b_k \sigma_+ + a_k^*(t_1) b_k^\dagger \sigma_-, \rho_S(t_1) \otimes \rho_E(0)]] \}. \quad (35)$$

since only $k = k'$ terms are non zero. Now we come face to face with a technical hurdle, we must now compute the 16 partial traces originating from the integrand in the above. We will simply proceed to the result but will display the fully expanded integrand bellow just to invoke appreciation for the level of complexity that arises in quantum open systems, even when the system, environment and the dynamics are as simple as we laid them out to be. The spontaneous emission model is virtually as simple as a quantum open system can get without becoming trivial.

$$\begin{aligned} & Tr_E \{ [(G_k(t) b_k \sigma_+ + G_k^*(t) b_k^\dagger \sigma_-), [(G_k(t_1) b_k \sigma_+ + G_k^*(t_1) b_k^\dagger \sigma_-), \rho_S(t_1) \otimes \rho_E(0)]] \} = \\ & = Tr_E (G_k(t) G_k(t_1) b_k^2 \sigma_+^2 \rho_S(t_1) \otimes \rho_E(0)) - Tr_E (G_k(t) G_k(t_1) b_k \sigma_+ \rho_S(t_1) \otimes \rho_E(0) b_k \sigma_+) \\ & \quad - Tr_E (G_k(t) G_k(t_1) b_k \sigma_+ \rho_S(t_1) \otimes \rho_E(0) b_k \sigma_+) + Tr_E (G_k(t) G_k(t_1) \rho_S(t_1) \otimes \rho_E(0) b_k^2 \sigma_+^2) \\ & \quad + Tr_E (G_k(t) G_k^*(t_1) b_k b_k^\dagger \sigma_+ \sigma_- \rho_S(t_1) \otimes \rho_E(0)) - Tr_E (G_k(t) G_k^*(t_1) b_k^\dagger \sigma_- \rho_S(t_1) \otimes \rho_E(0) b_k \sigma_+) \end{aligned}$$

$$\begin{aligned}
& -Tr_E(G_k(t)G_k^*(t_1)b_k\sigma_+\rho_S(t_1) \otimes \rho_E(0)b_k^\dagger\sigma_-) + Tr_E(G_k(t)G_k^*(t_1)\rho_S(t_1) \otimes \rho_E(0)b_k^\dagger b_k\sigma_-\sigma_+) \\
& +Tr_E(G_k^*(t)G_k(t_1)b_k^\dagger b_k\sigma_-\sigma_+\rho_S(t_1) \otimes \rho_E(0)) - Tr_E(G_k^*(t)G_k(t_1)b_k\sigma_+\rho_S(t_1) \otimes \rho_E(0)b_k^\dagger\sigma_-) \\
& -Tr_E(G_k^*(t)G_k(t_1)b_k^\dagger\sigma_-\rho_S(t_1) \otimes \rho_E(0)b_k\sigma_+) + Tr_E(G_k(t)G_k^*(t_1)\rho_S(t_1) \otimes \rho_E(0)b_k b_k^\dagger\sigma_+\sigma_-) \\
& +Tr_E(G_k^*(t)G_k^*(t_1)(b_k^\dagger)^2\sigma_-^2\rho_S(t_1) \otimes \rho_E(0)) - Tr_E(G_k^*(t)G_k^*(t_1)b_k^\dagger\sigma_-\rho_S(t_1) \otimes \rho_E(0)b_k^\dagger\sigma_-) \\
& -Tr_E(G_k^*(t)G_k^*(t_1)(b_k\sigma_+\rho_S(t_1) \otimes \rho_E(0)b_k^\dagger\sigma_-) - Tr_E(G_k^*(t)G_k^*(t_1)\rho_S(t_1) \otimes \rho_E(0)b_k b_k^\dagger\sigma_+\sigma_-).
\end{aligned}$$

Collecting the nonzero terms in the final expression one gets

$$\partial_t \rho_S(t) = - \int_0^t dt_1 \sum_k a_k(t) a_k^*(t_1) (\sigma_+ \sigma_- \rho_S(t_1) - \sigma_- \rho_S(t_1) \sigma_+) + h.c. \quad (36)$$

- h.c. is the *Hermitian* conjugate of the neighboring summand.

The term $\sum_k a_k(t) a_k^*(t_1)$ and its conjugate can be approximated by an integral due to our assumptions that the bath is large relative to our system and the system interacts equally with each of the virtually continuous degrees of freedom of the environment. Recalling how $a_k(t)$ was defined, our sum is approximated by

$$\Gamma(t - t_1) = \int_0^\infty d\omega P(\omega) g^2(\omega) e^{i(\omega_a - \omega)(t - t_1)}.$$

Here $P(\omega)$ is the density of the field modes as a function of frequency, and in practice the term $P(\omega)g^2(\omega)$ is smoothly varying in the vicinity of ω_a and therefore our integrand $\Gamma(t - t_1)$ is sharply peaked at $t = t_1$, this is an adaption of the version Wise et al man give in their book ??on quantum control . This means that we can approximate the term $\rho_S(t_1)$ by $\rho_S(t)$. The importance of this approximation just made here can not be overstated, this is what we have been working towards, it means that the integral term in our equation is now local in time. This is the *Markov* approximation in action.

$$\partial_t \rho_S(t) = -(\sigma_+ \sigma_- \rho_S(t) - \sigma_- \rho_S(t) \sigma_+) \int_{-\infty}^t dt_1 \Gamma(t - t_1) + h.c.. \quad (37)$$

We changed the lower limit of integration to $-\infty$ since the integrand $\Gamma(t - t_1)$ is negligible for values of t_1 varying significantly from t . I will make the substitution $\Delta\omega_a - i\frac{\gamma}{2} = -i \int_0^\infty dt_1 \Gamma(t - t_1)$ where $\Delta\omega_a$ is the frequency shift of the two level atom and γ is the radioactive decay of the atom [6]. With the above substitution and the definition $D[\sigma_-]\rho = \sigma_- \rho \sigma_+ - \frac{1}{2}(\sigma_+ \sigma_- \rho + \rho \sigma_+ \sigma_-)$ we can do one last modification to our differential equation. i.e.

$$\partial_t \rho_S(t) = \frac{-i}{2} \Delta\omega_a [\sigma_z, \rho_S(t)] + \gamma D[\sigma_-] \rho_S(t). \quad (38)$$

We may now revert back from the interaction picture.

$$\partial_t \rho_S(t) = \frac{-i}{2} (\omega_a + \Delta\omega_a) [\sigma_z, \rho_S(t)] + \gamma D[\sigma_-] \rho_S(t). \quad (39)$$

An equation of this form is called a *Born - Markov* Master equation, Lindblad Master equation and/or an equation of Lindblad form.

2.1.1 Solution

The most general form a the state matrix $\rho_S(t)$ can take is

$$\rho_S(t) = \frac{1}{2} [I_2 + x(t)\sigma_x + y(t)\sigma_y + z(t)\sigma_z] \quad (40)$$

Coherences are present via the σ_y and σ_x terms, we will therefore monitor decoherence via $x(t)$ and $y(t)$. The scalar functions $x(t)$, $y(t)$, and $z(t)$ are computed in the following way.

- $\frac{\partial}{\partial t} z(t) = Tr\{\sigma_z \frac{\partial}{\partial t} \rho_S(t)\}$

- $\frac{\partial}{\partial t} y(t) = Tr\{\sigma_y \frac{\partial}{\partial t} \rho_S(t)\}$
- $\frac{\partial}{\partial t} x(t) = Tr\{\sigma_x \frac{\partial}{\partial t} \rho_S(t)\}$

Using the *Lindblad* Master equation to substitute for $\frac{\partial}{\partial t} \rho_S(t)$ these equations become

- $\frac{\partial}{\partial t} z(t) = -\gamma(z(t) + 1)$
- $\frac{\partial}{\partial t} y(t) = (\Delta\omega_a)x(t) - \frac{\gamma}{2}y(t)$
- $\frac{\partial}{\partial t} x(t) = -(\Delta\omega_a)y(t) - \frac{\gamma}{2}x(t)$

with solutions

- $z(t) = 2e^{-\gamma t} - 1$
- $y(t) = -e^{-\frac{\gamma t}{2}} \sin((\omega_a + \Delta\omega_a)t)$
- $x(t) = e^{-\frac{\gamma t}{2}} \sin((\omega_a + \Delta\omega_a)t)$.

The solution to the *Lindblad* Master equation in the spontaneous emission case is therefore the following state matrix.

$$\rho_S(t) \rightarrow \begin{bmatrix} e^{-\gamma t} & e^{-\frac{\gamma t}{2}} \sin((\omega_a + \Delta_a)t) \frac{(1+i)}{2} \\ e^{-\frac{\gamma t}{2}} \sin((\omega_a + \Delta_a)t) \frac{(1-i)}{2} & 1 - e^{-\gamma t} \end{bmatrix} \quad (41)$$

Notice the exponential decay! This was to be expected! Also, notice the decoherence, i.e. the decay of the off-diagonal entries.

We have solved the Lindblad Master equation for a Two-Level atom in the vacuum. Now, we did this for a low dimensional quantum system. As the dimension N grows the number of coupled differential equations grows as $N^2 - 1$. For spin systems/ two-level systems the dimensionality $N = 2^n$ where n is the number of spins. This is a computational feat that is formidable at best. Methods that steer clear of the systems of differential equations approach are therefore of great interest. One such method is the so called Quantum-Jump Monte-Carlo method which is related to the so called unravellings in the theory of Quantum Stochastic Calculus. In what is to come we will briefly comment on Quantum unravellings and then move on to the Quantum Jump approach. For cases where the Lindbladian requires numerical methods to solve we may turn to the so called unravelling techniques which allow us to attain approximate solutions to the Lindblad master equation for a reduced cost.

3 The Stochastic Schrödinger equation and Quantum Jumps

Approximate solutions to the Lindblad master equation 22 may be obtained by solving a pertinent stochastic schrödinger equation. Deducing a stochastic schrödinger equation whose solutions are solutions to the relevant master equations is a process called unravelling in the literature and it is beyond the scope of this paper, for a great synopsis on the subject one may take a look at the paper by Petruccione and Moodley [12] One such unravelling is the so called Quantum Jumps unravelling [13] which is described by the stochastic schrödinger equation, let us consider the case with only one jump operator for simplicity.

$$|d\bar{\psi}\rangle = -iH_{eff}|\bar{\psi}\rangle dt + \frac{1}{2}\langle C^\dagger C \rangle |\bar{\psi}\rangle dt + \left(\frac{C}{\sqrt{\langle C^\dagger C \rangle}} - 1 \right) |\bar{\psi}\rangle dN, \quad (42)$$

above $|\bar{\psi}\rangle := |\psi\rangle/\sqrt{\langle\psi|\psi\rangle}$ and $H_{eff} = H_S - \frac{i}{2}C^\dagger C$, in general $H_{eff} = H_S - \frac{i}{2}\sum_n C_n^\dagger C_n$. This is a stochastic differential equation where dN is a stochastic variable which is 0 except at random times (corresponding to the jumps) when it becomes 1. It has statistics $dN dN = dN$, $M_{|\psi\rangle}(dN) = \gamma\langle C^\dagger C \rangle$ where $M_{|\psi\rangle}$ denotes the ensemble average over all trajectories which are in the state $|\psi\rangle$ at the time t . Note that this approach allows us to work with the state vectors as opposed to the corresponding density operators. This reduces complexity since the dimension of a density operator is the square of the dimension of its corresponding state vector. It turns out that there are an infinitum of ways to unravel the Lindblad master equation but we will stick to this one. This unravelling and the Monte Carlo wave-function are actually equivalent but often presented as stand alone approaches in the literature.

3.1 The Monte Carlo wave-function

Explicit invocation of the stochastic Schrödinger equation need not be made when utilizing the Quantum Jumps approach to approximate the solutions to the Lindblad master equation. This method is denominated the Monte Carlo wave-function and the schematic is the following [14].

The state-vector initial condition $|\psi(0)\rangle$ of a single trajectory is taken from an ensemble that appropriately samples the initial density operator $\rho_S(0)$ (in general, we need many state vectors from this ensemble and many trajectories for each state-vector initial condition). The Monte Carlo wave function method evolves $|\psi(t)\rangle$ to $|\psi(t + \delta t)\rangle$ as follows

1. To begin, the state vector is evolved according to the non-unitary dynamics afforded by the operator H_{eff} as described by the differential equation

$$i\partial_t|\psi\rangle = H_{eff}|\psi\rangle.$$

Neglecting terms of order δt^2 and higher $|\psi(t + \delta t)\rangle \approx (1 - iH_{eff}\delta t)|\psi(t)\rangle$. Owing to the fact that H_{eff} is not Hermitian, the evolved operator $|\psi(t + \delta t)\rangle$ is not normalized even if $|\psi(t)\rangle$ was to begin with. The normalization term reads

$$\langle\psi(t + \delta t)|\psi(t + \delta t)\rangle \approx 1 - \delta p$$

where $\delta p := \delta t i \langle\psi(t)|H_{eff} - H_{eff}^\dagger|\psi(t)\rangle$ where $|\psi(t)\rangle$ is normalized. Recall that $H_{eff} := H_S - \frac{i}{2} \sum_n C_n^\dagger C_n$ for the general case, which means that $H_{eff} - H_{eff}^\dagger = -2\frac{i}{2} \sum_n C_n^\dagger C_n = -i \sum_n C_n^\dagger C_n$. δp is therefore

$$\delta p = \delta t \langle\psi(t)| \sum_n C_n^\dagger C_n |\psi(t)\rangle \geq 0.$$

Notice that the time step δt must be small enough so that this first-order calculation be valid. Finding an appropriate δt is often the main hurdle to overcome in order to find faithful approximations to solutions of the Lindblad master equation in question. In some papers [14] it is required that $\delta p \ll 1$. This requirement is needed in order to insure that the probability of two jumps occurring in the same time step be negligible. This is a reasonable assumption for open systems where the system interacts weakly with its environment.

2. Here is the Monte Carlo aspect of the algorithm. A possible jump with total probability δp . Choose a random number α in $[0, 1]$, and if $\delta p < \alpha$ no jump occurs (this should be the case most of the time due to weak interaction) and the new normalized state at $t + \delta t$ is now

$$|\psi(t + \delta t)\rangle \Big|_{nojump} := \frac{(1 - iH_{eff}\delta t)}{\sqrt{1 - \delta p}} |\psi(t)\rangle.$$

Now, if $\alpha < \delta p$, a jump occurs, and the new normalized state vector is chosen from among the different state vectors $C_m|\psi(t)\rangle$ with probability distribution $\pi_m = \frac{\delta p_m}{\delta p}$ where $\delta p_m := \delta t \langle\psi(t)|C_m^\dagger C_m|\psi(t)\rangle$:

$$|\psi(t + \delta t)\rangle \Big|_{mthjump} = \frac{\sqrt{\delta t} C_m}{\sqrt{\delta p_m}} |\psi(t)\rangle.$$

The steps above can be shown to produce the Lindblad master equation to first order in δt if we average the evolved state of one trajectory. The algorithm above applies to state vectors but the corresponding density operators are obtained by taking the outer products of our state vectors with themselves. An average trajectory (of δt evolution) of a density operator is therefore computed as

$$\begin{aligned} \rho_{sys}(t + \delta t) &= |\psi(t + \delta t)\rangle \langle\psi(t + \delta t)| = (1 - \delta p) |\psi(t + \delta t)\rangle \langle\psi(t + \delta t)| \Big|_{nojump} + \sum_m \delta_m |\psi(t + \delta t)\rangle \langle\psi(t + \delta t)| \Big|_{mthjump} = \\ &= (1 - i\delta t H_{eff}) |\psi(t)\rangle \langle\psi(t)| \left(1 + \frac{i\delta t H_{eff}^\dagger}{\hbar}\right) + \delta t \sum_n C_n |\psi(t)\rangle \langle\psi(t)| C_n^\dagger = \end{aligned}$$

$$\begin{aligned}
|\psi(t)\rangle\langle\psi(t)| + \delta t \left(-iH_{eff}|\psi(t)\rangle\langle\psi(t)| + |\psi(t)\rangle\langle\psi(t)|iH_{eff}^\dagger \right) + \delta t \sum_n C_n |\psi(t)\rangle\langle\psi(t)|C_n^\dagger + O(\delta t^2) \approx \\
\rho_{sys}(t) + \delta t \left(-iH_{eff}\rho_{sys}(t) + i\rho_{sys}(t)H_{eff}^\dagger \right) + \delta t \sum_n C_n \rho_{sys}(t) C_n^\dagger = \\
\rho_{sys}(t) + \delta t \left(-i[H, \rho_{sys}(t)] - \frac{1}{2} \sum_n C_n^\dagger C_n \rho_{sys}(t) - \frac{1}{2} \sum_n \rho_{sys}(t) C_n^\dagger C_n \right) + \delta t \sum_n C_n \rho_{sys}(t) C_n^\dagger
\end{aligned}$$

This can be conclusively written as

$$\frac{\rho_{sys}(t + \delta t) - \rho_{sys}(t)}{\delta t} \approx -i[H, \rho_{sys}(t)] - \frac{1}{2} \sum_n C_n^\dagger C_n \rho_{sys}(t) - \frac{1}{2} \sum_n \rho_{sys}(t) C_n^\dagger C_n + \sum_n C_n \rho_{sys}(t) C_n^\dagger$$

which is equivalent to the Lindblad master equation 22 in the limit $\delta t \rightarrow 0$.

In the following section we will use the Quantum Jump technique in order to analyze the statistical behavior of the observable σ_z for a two level system in a the vacuum.

4 Monte Carlo wave function simulations

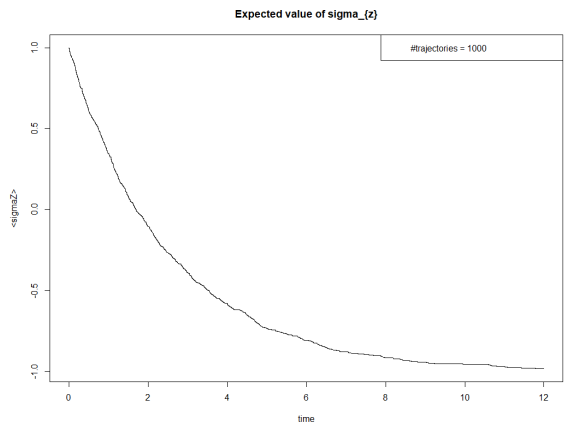
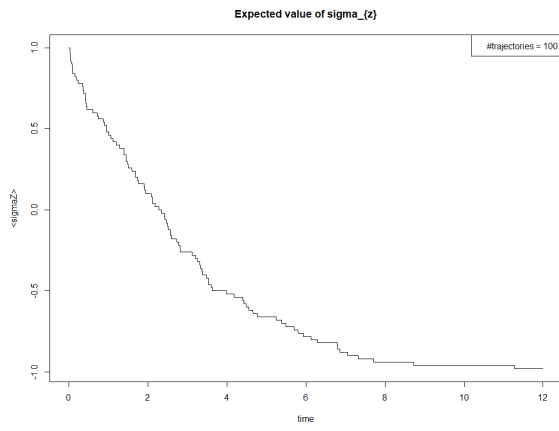
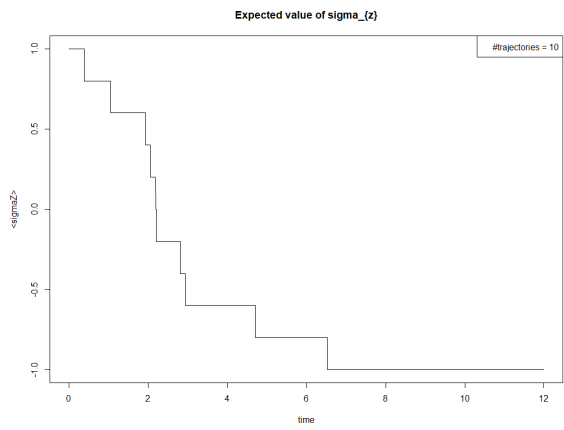
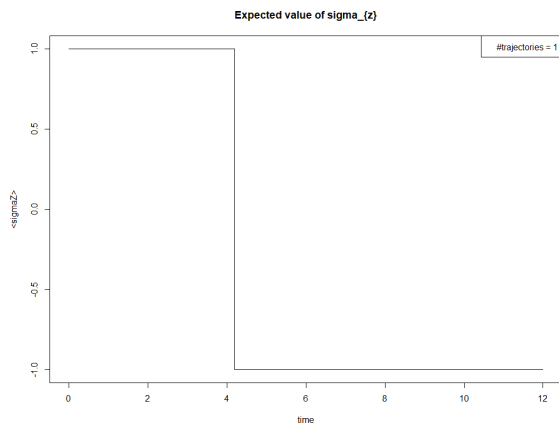
Let us now return to the master equation deduced in section 2 for a two level system in the vacuum. This master equation had the form

$$\partial_t \rho_S(t) = \frac{-i}{2} (\omega_a + \Delta\omega_a) [\sigma_z, \rho_S(t)] + \gamma D[\sigma_-] \rho_S(t). \quad (43)$$

where

$$D[\sigma_-] \rho = \sigma_- \rho \sigma_+ - \frac{1}{2} (\sigma_+ \sigma_- \rho + \rho \sigma_+ \sigma_-).$$

We will fix $\delta t = 0.001$, $\gamma = 0.1 = \omega_a$. We next implement the Quantum Jump Monte-Carlo program with use of the programming language R for a varying number of trajectories $N \in \{1, 10, 100, 1000\}$. My results are in the image block below. Notice the decay from spin up $\langle\sigma_z\rangle = 1$ to spin down $\langle\sigma_z\rangle = -1$. We



finally conclude this report by trying our hand at a model akin to the single two level system in a bath, namely a system of two coupled two level atoms in the vacuum. The relevant Master equation is quite similar to that of the single two level system in the vacuum.

$$\partial_t \rho_S(t) = \frac{-i}{2}(\omega_{a1} + \Delta\omega_{a1})[\sigma_{z1}, \rho_S(t)] + [J_x \sigma_x \otimes \sigma_x + J_y \sigma_y \otimes \sigma_y + J_z \sigma_z \otimes \sigma_z, \rho_S(t)] + \quad (44)$$

$$\frac{-i}{2}(\omega_{a2} + \Delta\omega_{a2})[\sigma_{z2}, \rho_S(t)] + \gamma \left\{ \Sigma_- \rho_S(t) \Sigma_+ - \frac{1}{2}(\Sigma_+ \Sigma_- \rho_S(t) + \rho_S(t) \Sigma_+ \Sigma_-) \right\}. \quad (45)$$

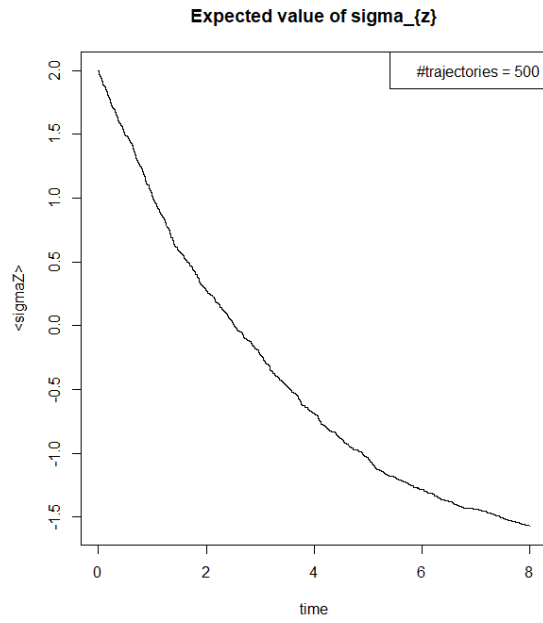
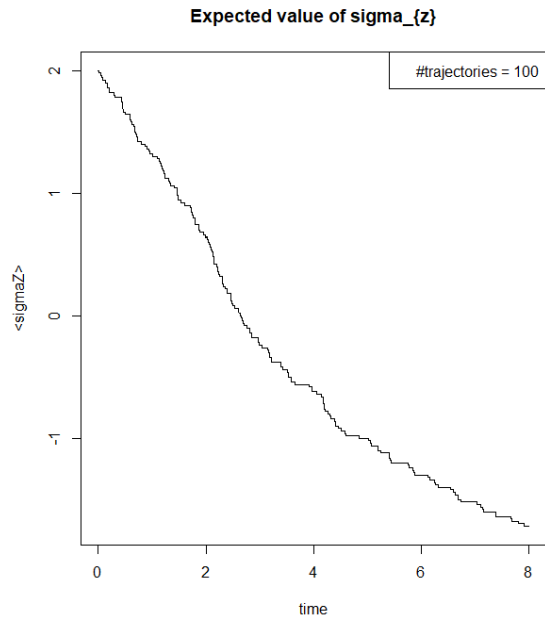
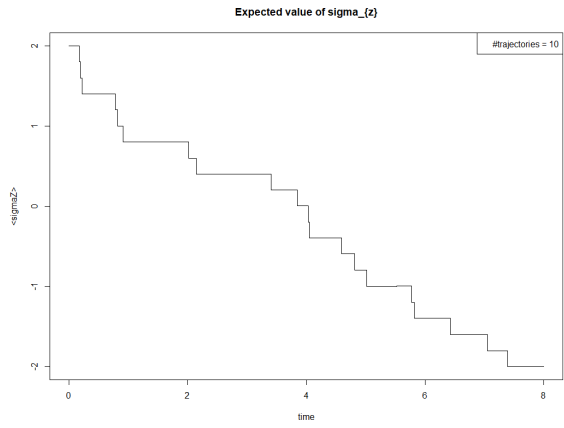
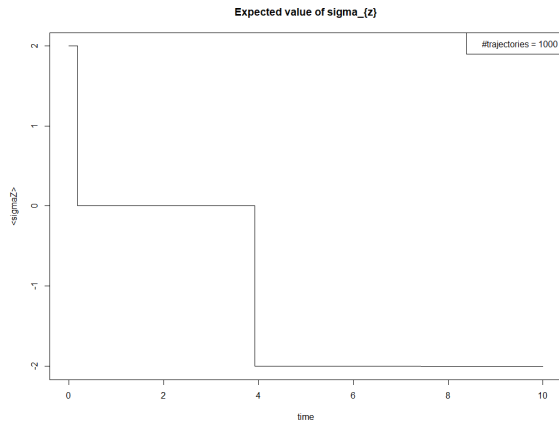
Where

- $\sigma_{z1} = \sigma_z \otimes I_2$
- $\sigma_{z2} = I_2 \otimes \sigma_z$
- $\Sigma_- = \sigma_- \otimes I_2 + I_2 \otimes \sigma_-$
- I_2 is the 2-D identity operator.

Fixing the relevant parameters as follows

- $\sigma_{a1} = \sigma_{a2} = \gamma = 0.1$
- $J_x = J_y = J_z = 0.2$
- $\delta t = 0.001$.

We will vary the trajectory parameter in the code as follows $N \in \{1, 10, 100, 500\}$ just like we did with the single spin simulation above. Instead of monitoring the observable σ_z we will monitor $\sigma_{z1} + \sigma_{z2}$ in this case. Note that the y-axis labels used for the graphs below are the same that were used for the graphs above. However, in the bottom case $\langle \text{sigmaZ} \rangle := \sigma_{z1} + \sigma_{z2}$. We have kept the title the same, i.e. Expected value of sigmaz but this should be understood here as total spin which is represented by $\sigma_{z1} + \sigma_{z2}$. We can not go as high as one thousand trajectories because for this to be the case I would have to sacrifice the smallness of δt which would yield poor results or I would have to constrain myself to a smaller time domain which will not allow me to truly appreciate the dynamics of the total spin observable. Notice the decay from both two level systems spin up $\langle \sigma_{z1} + \sigma_{z2} \rangle = 2$ to both two level systems spin down $\langle \sigma_{z1} + \sigma_{z2} \rangle = -2$.



5 conclusion

The Quantum Jumps for the single Two-Level and double Two-Level system were successful in the sense that they reproduced the expected exponential decay for the respective total spin observables. However, more analysis regarding the optimal δt to be used should be taken on since this was a great hurdle when selecting parameters for my simulations. The complexity of the program I have written grows with respect to the size of my time domain partitioning and number of trajectories since I use an N by cardinality (Timedomain) matrix in my code in order to implement the Quantum Jump method. Perhaps a better way, one avoiding matrices may be adopted.

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