

MONTE CARLO SIMULATIONS IN  
OPEN QUANTUM SYSTEMS

by

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## ABSTRACT

The motivation for this Masters thesis is to develop numerical algorithms to study the dynamical evolution of non-Markovian open quantum systems. Such systems are of importance if one is interested in modeling solid state systems which are candidates for the qubit - the quantum analog of the binary digit. Such an example may be a trapped spin onto which is encoded a chosen spin state. In reality, such a spin is never completely isolated from the environment, and so from a practical point of view it is of interest to study the dynamics of this interaction between some open system with an environment. The goal here is to create a computer program to simulate this behaviour of all density matrix elements for the open system numerically. Many interesting quantum systems, spin chains as an example, do not behave as a Markovian process, and it is sometimes difficult or perhaps indeed impossible to derive exact analytical solutions. As such, the techniques used in this thesis are aimed at describing non-Markovian processes in a way that approaches the exact solution.

The study begins by introducing the reader to important concepts and results in the general study of both closed and open quantum systems. Differences in the treatment of the two types of systems are pointed out, and the necessary standard equations used generally are presented. Additionally, two different techniques are explained for the study of open quantum systems, namely the density matrix approach and the stochastic wavefunction approach. Important results from these two methods are presented and the section ends by convincing the reader of their equivalence.

The second chapter begins with an example of an open quantum system which exhibits non-Markovian behaviour. The model of the spin star system is described and important results are given from references. This chapter introduces the reader to the model, conceptually explaining the system, and going on to show its exact analytical behaviour. This basic model, with minor changes, will be used throughout this study and the physics, interactions and symmetries, does not really change.

This study then shows how one can use the stochastic wavefunction method to solve the dynamics of the spin star model. This chapter follows with deriving stochastic equations for the same system as the preceding chapter, and using these equations a numerical algorithm is developed, the results of which provide a good comparison between the exact analytical and exact numerical techniques.

As a further example, a similar but slightly more complex system is studied in exactly the same manner, with the only important difference being that the open quantum system to be modeled is now a spin-one particle. Important differences in the results are pointed out and explained, and important similarities are highlighted. In presenting the results of this second simulation, shortcomings of the numerical technique and areas of applicability are discussed.

In the final chapter the author considers using this numerical technique's ability to completely map the dynamics for a density matrix to investigate a measure of quantumness for an open system. This research has been submitted for publication to a peer reviewed journal.

## PREFACE

All research in this Masters thesis was carried out at the School of Physics, University of KwaZulu-Natal, Westville Campus, from the period March 2005 to September 2007, under the supervision of Professor Francesco Petruccione.

These studies represent original work by the author and have not otherwise been submitted in any form for any other degree or diploma to any other tertiary institution. Where use has been made of the work of others it is duly acknowledged in this text.

Signed: \_\_\_\_\_



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## 1. INTRODUCTION

“There is nothing new to be discovered in physics now. All that remains is more and more precise measurement.” In an address to the British Association for the Advancement of Science in the year 1900, Lord Kelvin’s statement couldn’t have been farther from the truth. In another address to the Royal Institution of Great Britain, Lord Kelvin would describe the two remaining questions left to resolve before the field of physics was completely understood. The first question was the mathematical modeling of the spectrum of blackbody radiation, and the second was the strange conclusion of the Michelson-Morley experiment.

Albert Michelson and Edward Morley set up an interferometer to test for the existence of “Æther”, which was postulated to be the medium in which electromagnetic waves propagate. From the results of their experiment, it was concluded that this æther does not exist, and so raised more questions as to the nature of light.

Newtonian physics could not explain the theory of blackbody radiation. The problem was that the classical equations of physics at the time led to the so-called “ultraviolet catastrophe” - the intensity of light emitted from a perfect absorber, a blackbody, would approach infinity as the frequency approached infinity [1]. As it was experimentally known that the measured intensity had a maximum, this posed a problem for the physicists of the time.

From these two seemingly innocent problems grew the fields that we now know as Special Relativity and Quantum Mechanics. The problem of the ultraviolet catastrophe was solved by exploring the hypothesis put forward earlier by Max Planck, that electromagnetic radiation could only be emitted or absorbed in discrete packets, or quanta, proportional to the frequency. This hypothesis led Albert Einstein to postulate that light itself consisted of discrete individual quanta, and received a Nobel prize for his work on the photoelectric effect [2]. These quanta of light would later become known as photons. The story of the development of quantum mechanics may be found in [3].

From humble beginnings, the field of Quantum Mechanics rapidly grew over the

last century to become one of the most important areas of research in physics today. Without it, almost all modern conveniences would be an impossible dream. Electronics and modern medicine are just two examples of what would be impossibilities today without the revolutionary thinking that led to the birth of Quantum Mechanics. Examples of current technology in use all over the world thanks to Quantum Mechanics are the laser, magnetic resonance imaging devices in hospitals and the transistor.

With the invention of the transistor, giant calculating machines were rapidly miniaturised into the modern computers in use today. As transistors get smaller and smaller, current technology will approach a limit of what is possible without taking into account quantum effects. A growing area of interest in quantum mechanics is that of quantum information theory, or quantum computing [4]. This involves the amalgamation of the well developed field of information theory and computer science with quantum mechanics resulting in new algorithms for computation, means of communicating or storing data, and perhaps many as yet undiscovered applications. Examples of quantum computing algorithms include Shor's factorisation algorithm [5] and Grover's search algorithm [6]. An excellent reference on quantum information processing and computation can be found in [7]. Another popular topic of research is quantum encryption, or more correctly named quantum key distribution, making use of the laws of quantum mechanics to achieve absolutely secure communication channels [8].

The power of algorithms based on controlling quantum states in a useful way is due to the fact that a quantum state may exist in a superposition of possible states with probabilities. It is this unique feature of quantum states that have inspired many scientists to come up with new and innovative methods of processing information which would take much longer using more traditional techniques. Moreover, one may manipulate quantum states in such a way as to "entangle" [9] them, that is to introduce a correlation that is much stronger than the classical laws of statistics allow.

With the development of many useful quantum algorithms, the challenge is now to implement them. A major hurdle in implementing a working quantum computer is the rapid decoherence of the coherent quantum states used in storing and processing information. This study investigates a numerical technique used to model these decoherence effects, and so perhaps better understand how to avoid or control quantum systems in a useful way.

The numerical techniques presented in this study are based on the well known Monte Carlo method. Whilst the Monte Carlo method used in this study is quite simple, there are many much more complicated implementations [10] such as Quantum Optical Monte Carlo techniques and the Monte Carlo Markov Chain method [11]. These more complex variations on the standard Monte Carlo method are necessary for some particularly complex models, but in the case of this study the most basic knowledge will suffice.

The Monte Carlo method is employed to suitably generate a random distribution of inputs for a numerical calculation. As an example, the value of Pi can be calculated by simulating a number of darts thrown at a square board with sides of unit length. The distribution of the points where each dart strikes the board should be uniform. After simulating a large number of such throws, Pi can be approximated as the ratio of the number of darts landing inside a unit circle centred inside the square board versus the total number of darts thrown. The Monte Carlo method is simply the averaging over many realisations of a dart thrown with a uniform distribution.

Monte Carlo simulations may be employed, for example, to solve for the energy levels in the Hydrogen atom. This is essentially a static problem, and modeling dynamic models is much more interest. Of particular interest is the modeling of the density matrix for a quantum state. As an example, Monte Carlo simulations can be used to simulate the time evolution of quantum states by the stochastic wavefunction method. This shall be explained in more detail in Chapter 1.3

### 1.1 Closed Quantum Systems

The typical study of a quantum system is that of a closed system. An example of such a system is illustrated by Figure 1.1. In this figure, there is the closed system of interest embedded in an environment. The important feature of a closed system is that there is absolutely no interaction between it and the environment - the closed system is completely insulated from any and all outside influences. In Nature, the only true completely closed system is the universe itself, but for practical purposes it is nevertheless useful to build models of closed systems composed perhaps of just one particle, a cloud of atoms, or a number of photons. These models can give useful predictions of the behaviour of phenomena when looking at timescales much shorter than the time it would take for any quantum effects to “leak” out into the environment, or when coupling to the environment is very weak. Although it is a

very important starting point, more interesting phenomena needs to be treated as an open quantum system, which will be introduced later. Many excellent books on the study of quantum systems are available, some examples are [12], [13] and [14].

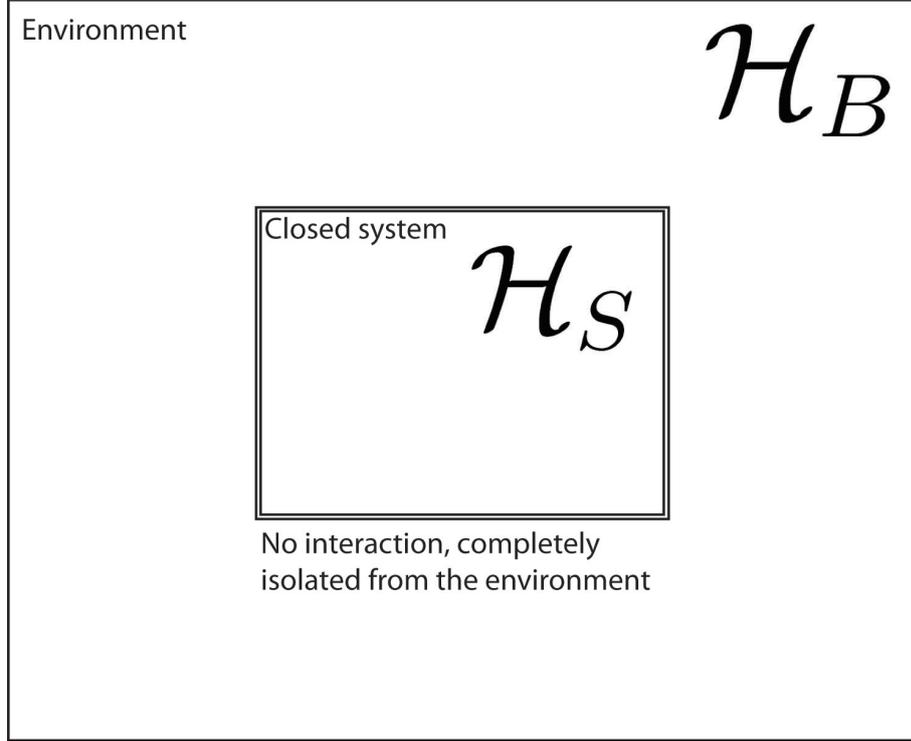


Fig. 1.1: A diagram representing a closed quantum system, where the system of interest is completely isolated from any environment.

A state in quantum mechanics is represented using Dirac's bra-ket notation [15] as the ket vector  $|\psi\rangle$ . Using the Schrödinger equation, the time evolution of a quantum state is written as

$$\frac{d}{dt} |\psi(t)\rangle = \frac{-i}{\hbar} H(t) |\psi(t)\rangle. \quad (1.1)$$

In the above equation,  $H(t)$  is the time dependent Hamiltonian for the system and  $\hbar$  is Planck's constant which shall henceforth be set equal to 1. In order to write a solution to this equation, a unitary time evolution operator  $U(t, t_0)$  is introduced which acts on some initial state vector  $|\psi(0)\rangle$  to give the equation

$$|\psi(t)\rangle = U(t, t_0) |\psi(0)\rangle, \quad (1.2)$$

with the condition that

$$U(t_0, t_0) = I. \quad (1.3)$$

Substituting Equation (1.2) back into Schrödinger's equation (1.1) results in the following equation for the time evolution operator;

$$\frac{\partial}{\partial t} U(t, t_0) = -iH(t)U(t, t_0). \quad (1.4)$$

Using the above two equations, it can be seen that for a closed system where the Hamiltonian is not time dependent the evolution operator can be written in the form

$$U(t, t_0) = \exp(-iH(t)(t - t_0)), \quad (1.5)$$

and it follows immediately that

$$U(t, t_0)U^\dagger(t, t_0) = U^\dagger(t, t_0)U(t, t_0) = I, \quad (1.6)$$

and hence that  $U(t, t_0)$  is unitary.

More generally, the mixed state of a quantum system is represented using a statistical operator called the density matrix  $\rho$ . The density matrix for a mixed state of a closed system is defined as

$$\rho = \sum_j p_j |\psi_j\rangle \langle \psi_j|, \quad (1.7)$$

where  $\rho$  represents a mixed ensemble of states  $|\psi_j\rangle$ , and  $p_j$  are their corresponding probability weights. These weights are positive and sum to unity:

$$p_j \geq 0, \quad (1.8)$$

$$\sum_j p_j = 1. \quad (1.9)$$

It is also a requirement that the trace of a density matrix be 1, and the density matrix is a positive hermitian operator:

$$\text{Tr}\{\rho(t)\} = 1, \quad (1.10)$$

$$\rho(t) = \rho^\dagger(t), \quad (1.11)$$

$$\rho(t) \geq 0. \quad (1.12)$$

Through these definitions, one can see that the density matrix is a positive semidefinite matrix and is self adjoint. It is used in studying the more general mixed states, and  $\rho = \rho^2$  if and only if  $\rho$  is a pure state.

Just as one can study the dynamics of a system's state vector, a set of equations can also be derived to model the dynamics of a system's density matrix. Using the definition of the density matrix (1.7), one can write

$$\rho(t) = \sum_j p_j U(t, t_0) |\psi_j(0)\rangle \langle \psi_j(0)| U^\dagger(t, t_0). \quad (1.13)$$

Taking the derivative of the above equation, and Equation (1.4), an expression for the dynamics of the density matrix is found:

$$\begin{aligned} \frac{d}{dt}\rho(t) &= \frac{d}{dt} \sum_j p_j U(t, t_0) |\psi_j(0)\rangle \langle \psi_j(0)| U^\dagger(t, t_0), \\ &= \sum_j p_j \frac{\partial}{\partial t} U(t, t_0) |\psi_j(0)\rangle \langle \psi_j(0)| U^\dagger(t, t_0) \\ &\quad + \sum_j p_j U(t, t_0) |\psi_j(0)\rangle \langle \psi_j(0)| \frac{\partial}{\partial t} U^\dagger(t, t_0), \\ &= \frac{\partial}{\partial t} U(t, t_0) \rho(0) U^\dagger(t, t_0) + U(t, t_0) \rho(0) \frac{\partial}{\partial t} U^\dagger(t, t_0), \\ &= -iH(t)U(t, t_0)\rho(0)U^\dagger(t, t_0) - iU(t, t_0)\rho(0)U^\dagger(t, t_0)H(t), \\ &= -iH(t)\rho(t) - i\rho(t)H(t). \end{aligned} \quad (1.14)$$

The above equation can now be written in a concise form;

$$\frac{d}{dt}\rho(t) = -i[H(t), \rho(t)], \quad (1.15)$$

where the square brackets represents the commutator  $[A, B] = AB - BA$ . The time evolution equation for the density matrix is commonly written as

$$\frac{d}{dt}\rho(t) = \mathcal{L}(t)\rho(t), \quad (1.16)$$

where the superoperator  $\mathcal{L}$ , the Liouville operator or Liouvillean, is defined as the

commutator brackets such that

$$\mathcal{L}(t)X(t) = [H(t), X(t)]. \quad (1.17)$$

The equation above is called the Liouville-von Neumann equation and is the master equation for a closed quantum system with a time dependent Hamiltonian. This is a first order differential equation governing the dynamics of the density matrix, and hence the time evolution of the probability of the system to occupy a set of states. In the case where the Hamiltonian is time independent, Equation (1.16) can be integrated giving

$$\rho(t) = \exp(\mathcal{L}t)\rho(0). \quad (1.18)$$

The equation (1.18) above is the general solution for the Liouville equation for a time independent Hamiltonian and will be used later in the model in Chapter 2.

## 1.2 The Density Matrix Approach to Open Quantum Systems

Much research has been conducted in the last century in advancing the theory of quantum mechanics, but it is only relatively recently that attention has been paid to what is known as “open quantum systems”. The traditional treatment of a quantum system is that of considering the system to be closed, or completely insulated from the environment. However, this is only a theoretical idealisation which almost never occurs in reality. Almost every system of practical interest is what can be called an open system, that is there exists at least some coupling with the outside world. It is this coupling to the environment which is of interest in this study. There are many good books on the subject of Open Quantum Systems, such examples are [16] and [17].

Difficulties in realising practical implementations of devices based on quantum mechanics arise in part from their interaction with the environment. Information which is stored in some quantum state may, for example, leak out into the environment through some coupling which has either not been taken into consideration or perhaps may even be unavoidable. If this process of information loss, or quantum decoherence [18], can be more fully understood, it may pave the way for more advanced implementations of quantum technologies to be realised. This is due to the fact that quantum devices make use of the coherent properties of quantum states in superposition. A loss of coherence results in a loss of data or an error in communication.

The state of the open system decoheres through some interaction with an outside system, where some part of the quantum state of interest 'leaks' in a thermodynamically irreversible way into the environment. In the case of an open quantum system, the master equation of the Liouville form is no longer sufficient to describe the time evolution of the system and the effects of dissipation and decoherence.

In general, the total system consists of the open system,  $S$ , which is coupled to some environment,  $B$ , through some interaction Hamiltonian  $H_I(t)$ . The environment  $B$  exists in the Hilbert space  $\mathcal{H}_B$ , and the open system  $S$  exists in the Hilbert space  $\mathcal{H}_S$ . As such, the density matrix of the total system exists in the combined Hilbert space,

$$\rho(t) \in \mathcal{H}_S \otimes \mathcal{H}_B. \quad (1.19)$$

The density matrix for the reduced system, the open system, can be calculated by taking the trace over the environment degrees of freedom giving

$$\begin{aligned} \rho_S(t) &= \text{Tr}_B\{\rho(t)\} \\ &= \text{Tr}_B\{U(t,0)\rho(0)U^\dagger(t,0)\}, \end{aligned} \quad (1.20)$$

where now the reduced system exists in the Hilbert space

$$\rho_S(t) \in \mathcal{H}_S. \quad (1.21)$$

Additionally, one can suppose the initial condition

$$\rho(0) = \rho_S(0) \otimes \rho_B(0), \quad (1.22)$$

where the initial state of the total system is just the tensor product of the initial state of the open system with the initial state of its environment. Another way to say this is to require that at the initial time  $t = 0$ , the open system is not entangled with its environment. The time taken for an open system to decohere, in other words the quantum information has 'leaked' into the environment, is known as the decoherence time. It is this time for an open system to decohere that is of practical importance when trying to realise quantum devices for real world applications. It is of great importance that decoherence and dissipation processes are modeled and understood, as these are the greatest hurdles to developing a means of robustly storing quantum information. This is because the information stored as quantum states exists only as

long as the quantum states themselves do not decohere. It is this coherence time that should be as long as possible - long enough to process in a useful way.

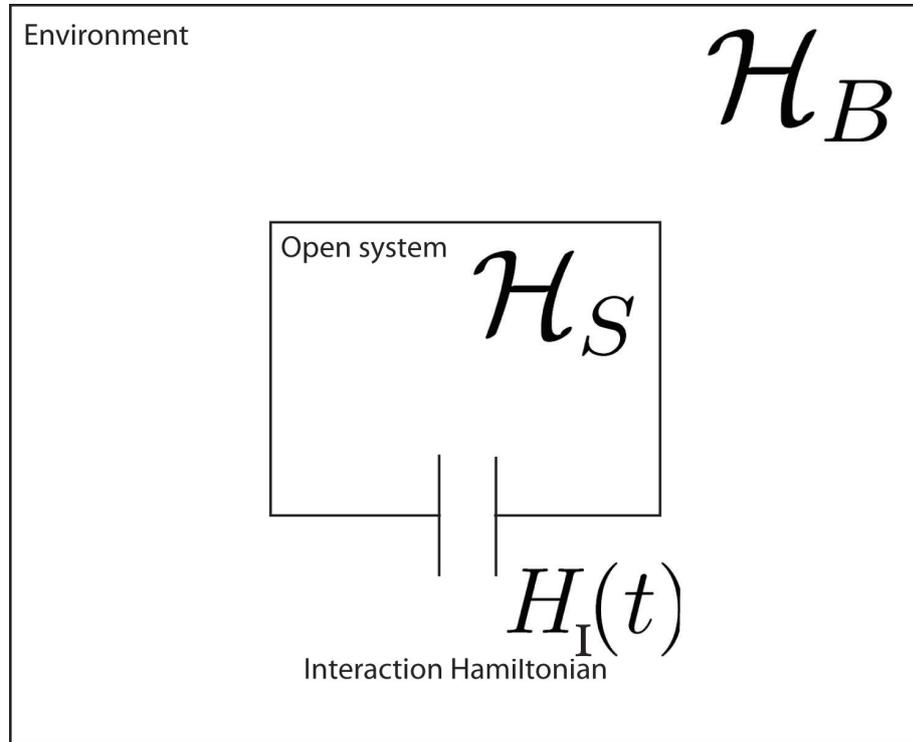


Fig. 1.2: A diagram representing an open quantum system, where the system of interest interacts with an environment through some interaction Hamiltonian.

To construct a master equation describing the dynamics of the reduced density matrix  $\rho_S(t)$ , one makes use of a dynamical map

$$V(t) : \mathcal{H}_S \rightarrow \mathcal{H}_S, \quad (1.23)$$

where the dynamical map  $V(t)$  consists of operators within the open system's Hilbert space  $\mathcal{H}_S$ . The most general form of the master equation for an open quantum system is found through the most general form of a generator of a quantum dynamical

semigroup, details of which can be found in [16]. This master equation is written as

$$\begin{aligned} \frac{d}{dt}\rho_S(t) &= -i[H(t), \rho_S(t)] \\ &+ \sum_{k=1}^{N^2-1} \gamma_k \left( A_k \rho_S(t) A_k^\dagger - \frac{1}{2} A_k^\dagger A_k \rho_S(t) - \frac{1}{2} \rho_S(t) A_k^\dagger A_k \right), \end{aligned} \quad (1.24)$$

and is known as the Lindblad equation. In this equation, the operators  $A_k$  are known as Lindblad operators which are taken to be linear combinations of a complete set of orthonormal basis vectors of the Liouville space having dimension  $N^2$  which corresponds to the open system's Hilbert space  $\mathcal{H}_S$  of dimension  $N$ . These Lindblad operators are dimensionless and the coefficients  $\gamma_k$  have units of inverse time.

One may note that the Lindblad equation is an extension of the Liouville equation presented in the previous section. In contrast to the Liouville equation, the Lindblad equation contains dissipative terms which account for the decoherence and dissipation of the open system. The Lindblad equation may also be written in the form

$$\frac{d}{dt}\rho_S(t) = -i[H(t), \rho_S(t)] + \mathcal{D}(\rho_S(t)), \quad (1.25)$$

where  $\mathcal{D}(\rho_S(t))$  represents the dissipative terms given above and is sometimes referred to as the dissipator. This master equation for Markovian open quantum systems models the dynamics of an open system including decoherence effects. This method of modelling the dynamics of a density matrix is not particularly useful for numerical simulations, but is used to analytically solve equations of motion which will be shown in Chapter 2. The following section describes an alternate method of modeling density matrices of open systems using a stochastic wavefunction approach.

### 1.3 The Stochastic Wavefunction Approach to Open Quantum Systems

One can describe the dynamics of the open system in terms of stochastic wavefunctions. In this section, it is supposed that the open system exists in some initial state  $|\psi(0)\rangle \in \mathcal{H}_S$ . This system undergoes time evolution through a process known as a piecewise deterministic process. This process is characterised by the system undergoing unitary, deterministic evolution, interrupted at random times by discrete jumps to some other state. It is required that both the unitary evolution and the jump process preserves the norm of the state vector, and the system begins in a known initial

state. Presented here is an argument showing how this description is equivalent to the density matrix approach from the previous section by recovering the Lindblad equation.

The master equation for the open system can be recovered from the stochastic differential equations for the state as follows. One begins with the stochastic differential equation for the open system's state:  $|\psi(t)\rangle$

$$d|\psi(t)\rangle = -iG(|\psi(t)\rangle)dt + \sum_i \left( \frac{A_i |\psi(t)\rangle}{\|A_i |\psi(t)\rangle\|} - |\psi(t)\rangle \right) dN_i, \quad (1.26)$$

where  $A$  is a the random jump operator[16]. The deterministic time evolution is given by

$$G(|\psi(t)\rangle) = \hat{H}(|\psi(t)\rangle) + \frac{i}{2} \sum_i \gamma_i \|A_i |\psi(t)\rangle\|^2 |\psi(t)\rangle$$

and the non-Hermitian operator which includes the Hamiltonian

$$\hat{H} = H - \frac{i}{2} \sum_i \gamma_i A_i A_i^\dagger.$$

With this, one can write, remembering that  $dN_i$  are Poisson increments and  $\gamma_i$  are the jump rates in the random jump process,

$$\begin{aligned} d|\psi(t)\rangle &= -iH |\psi(t)\rangle dt - \frac{1}{2} \sum_i \gamma_i A_i^\dagger A_i |\psi(t)\rangle dt \\ &\quad + \frac{1}{2} \sum_i \gamma_i \|A_i |\psi(t)\rangle\|^2 |\psi(t)\rangle dt \\ &\quad + \sum_i \left( \frac{A_i |\psi(t)\rangle}{\|A_i |\psi(t)\rangle\|} - |\psi(t)\rangle \right) dN_i. \end{aligned} \quad (1.27)$$

The statistics of the Poisson increments  $dN$  are such that  $dN_i dN_j = \delta_i^j dN_i$  and

$$E[dN_i] = \gamma_i \|A_i |\psi(t)\rangle\|^2 dt. \quad (1.28)$$

This means that only one Poisson increment is non-zero at any time.

In the following the aim is to derive an equation describing the dynamics of the density matrix  $\rho(t)$ . The expectation operator  $E[X]$  is defined as taking an average over a statistical ensemble  $X$ . Taking the expectation over the bath degrees of freedom

in the equation for the density matrix

$$\rho(t) = |\psi(t)\rangle \langle\psi(t)|, \quad (1.29)$$

leads to an equation for the density matrix of the open system:

$$\rho_S(t) = E[|\psi(t)\rangle \langle\psi(t)|]. \quad (1.30)$$

Using Equation (1.30) allows one to write  $\rho(t)$  in differential form. Using the product rule one can write

$$d\rho(t) = E[d|\psi(t)\rangle \langle\psi(t)| + |\psi(t)\rangle d\langle\psi(t)| + d|\psi(t)\rangle d\langle\psi(t)|]. \quad (1.31)$$

The action of taking the expectation is linear, hence the equation above can be written as

$$d\rho(t) = E[d|\psi(t)\rangle \langle\psi(t)|] + E[|\psi(t)\rangle d\langle\psi(t)|] + E[d|\psi(t)\rangle d\langle\psi(t)|]. \quad (1.32)$$

If the expression for  $d|\psi\rangle$  from (1.27) is inserted into (1.32) one gets

$$\begin{aligned}
d\rho(t) = & E[-iH|\psi(t)\rangle\langle\psi(t)|dt] \\
& -E\left[\frac{1}{2}\sum_i\gamma_iA^\dagger A|\psi(t)\rangle\langle\psi(t)|dt\right] \\
& +E\left[\frac{1}{2}\sum_i\gamma_i\|A_i|\psi(t)\rangle\|^2|\psi(t)\rangle\langle\psi(t)|dt\right] \\
& +E\left[\sum_i\left(\frac{A_i|\psi(t)\rangle\langle\psi(t)|}{\|A_i|\psi(t)\rangle\|}-|\psi(t)\rangle\langle\psi(t)|\right)dN_i\right] \\
& +E[|\psi(t)\rangle\langle\psi(t)|Hidt] \\
& -E\left[\frac{1}{2}\sum_i\gamma_i|\psi(t)\rangle\langle\psi(t)|A^\dagger Adt\right] \\
& +E\left[\frac{1}{2}\sum_i\gamma_i\|A_i|\psi(t)\rangle\|^2|\psi(t)\rangle\langle\psi(t)|dt\right] \\
& +E\left[\sum_i\left(\frac{|\psi(t)\rangle\langle\psi(t)|A_i}{\|A_i|\psi(t)\rangle\|}-|\psi(t)\rangle\langle\psi(t)|\right)dN_i\right] \\
& +E\left[\sum_i\left(\frac{A_i|\psi(t)\rangle}{\|A_i|\psi(t)\rangle\|}-|\psi(t)\rangle\right)dN_i\times\sum_j\left(\frac{\langle\psi(t)|A_j^\dagger}{\|A_j|\psi(t)\rangle\|}-\langle\psi(t)|\right)dN_j\right]
\end{aligned} \tag{1.33}$$

In the last term in the equation above all terms of order  $dt^2$  and higher are ignored. Using Equation (1.28), the three terms in the expectation in Equation (1.33) which each involve Poisson increments can be written as

$$\begin{aligned}
& \sum_i\gamma_iE\left[\left(\|A_i|\psi(t)\rangle\|A_i|\psi(t)\rangle\langle\psi(t)|-\|A_i|\psi(t)\rangle\|^2|\psi(t)\rangle\langle\psi(t)|\right.\right. \\
& \left.+\|A_i|\psi(t)\rangle\| |\psi(t)\rangle\langle\psi(t)|A_i-\|A_i|\psi(t)\rangle\|^2|\psi(t)\rangle\langle\psi(t)|\right. \\
& \left.+A_i|\psi(t)\rangle\langle\psi(t)|A_i^\dagger-A_i|\psi(t)\rangle\langle\psi(t)|\|A_i|\psi(t)\rangle\| \right. \\
& \left.-|\psi(t)\rangle\langle\psi(t)|A_i^\dagger\|A_i|\psi(t)\rangle\|+\|A_i|\psi(t)\rangle\|^2|\psi(t)\rangle\langle\psi(t)|\right)dt\Big]. \tag{1.34}
\end{aligned}$$

Now using the fact that the expectation function  $E[XY] = E[X]E[Y]$  if  $X$  and  $Y$  are independent and uncorrelated, (1.34) is substituted back into (1.33) giving

$$\begin{aligned} \frac{d\rho(t)}{dt} &= E[-iH |\psi(t)\rangle \langle\psi(t)| + |\psi(t)\rangle \langle\psi(t)| Hi \\ &\quad - \frac{1}{2} \sum_i \gamma_i A^\dagger A |\psi(t)\rangle \langle\psi(t)| - \frac{1}{2} \sum_i \gamma_i |\psi(t)\rangle \langle\psi(t)| A^\dagger A \\ &\quad + \sum_i \gamma_i A_i |\psi(t)\rangle \langle\psi(t)| A_i^\dagger. \end{aligned}$$

Finally taking expectations one arrives at

$$\frac{d\rho(t)}{dt} = -i[H, \rho(t)] + \sum_i \gamma_i \left( A_i \rho(t) A_i^\dagger - \frac{1}{2} A^\dagger A \rho(t) - \frac{1}{2} \rho(t) A^\dagger A \right), \quad (1.35)$$

recovering the Lindblad equation describing the dynamics of the open system. This shows that the description of the system in terms of a continuous drift process combined with finite random jumps is completely equivalent to the standard Lindblad master equation for the open system.

This approach to modeling open systems lends itself much more naturally to numerical simulations due to the relative simplicity of the deterministic drift and discrete jump processes compared with a master equation of the Lindblad type which contains dissipative terms that frequently are quite complex. Discussed thus far are means to model an open quantum system evolving as a Markov process. That is, the state of the system at a particular time depends only upon the previous state and not on the entire history of the state. Presented in the following chapter is a physical example which exhibits non-Markovian behaviour, and this model will be used throughout this study.

## 2. A NON-MARKOVIAN EXAMPLE OF AN OPEN QUANTUM SYSTEM

### 2.1 *The spin star Model*

The model in this study is known as a spin star model consisting of a number of spin one-half particles in a particular geometric configuration - one central spin surrounded by a bath of spins in a star configuration. The geometry of the model has the advantage that whilst displaying the behaviour one is interested in when studying open quantum systems, its dynamics can be solved for exactly, if the Hamiltonian is chosen appropriately, due to the high degree of symmetry.

In this study,  $N + 1$  spins are modeled, one central spin is surrounded by  $N$  bath spins. Each of the bath spins interacts independently with the central spin via the Heisenberg XY interaction. The interaction Hamiltonian for this interaction is given by

$$H = 2\lambda(\sigma_+ J_- + \sigma_- J_+). \quad (2.1)$$

In the above Hamiltonian,  $\lambda$  is a coupling constant which represents the strength of the interactions of the central spin with the environment spins. The  $\sigma_+$  and  $\sigma_-$  operators represent the raising and lowering operators respectively for the central spin. Expressing these in terms of the Pauli matrices gives

$$\sigma_{\pm} = \frac{1}{2}(\sigma_x \pm i\sigma_y), \quad (2.2)$$

where the familiar Pauli matrices are written as

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (2.3)$$

Similarly, the  $J_+$  and  $J_-$  operators are the raising and lowering operators for the bath, or environment, state given by the collective sum of the individual bath spin ladder

operators as

$$J_{\pm} = \sum_{r=1}^N \sigma_{\pm}^{(r)}, \quad (2.4)$$

where for each of the  $N$  bath spins

$$\sigma_{\pm}^{(r)} = \frac{1}{2}(\sigma_x^{(r)} \pm i\sigma_y^{(r)}). \quad (2.5)$$

Using this notation it can be said that the central spin's state vector, and its corresponding ladder operators,  $\sigma_+$  and  $\sigma_-$ , exist in the Hilbert space  $\mathcal{H}_S$ . The bath, or environment, state vector exists in the Hilbert space  $\mathcal{H}_B$ , which is made up of the  $N$ -fold tensor product of similar two dimensional  $\mathcal{H}_S$  spaces. As a consequence of this, the entire system, the bath and the central spin, exist in the Hilbert space given by  $\mathcal{H}_S \otimes \mathcal{H}_B$ .

In order to study the dynamics of the density matrix for this system, the solution of the Liouville-von Neumann equation

$$\frac{d}{dt}\rho(t) = \lambda\mathcal{L}\rho(t) \quad (2.6)$$

is written as

$$\rho(t) = e^{\lambda\mathcal{L}t}\rho(0), \quad (2.7)$$

where  $\mathcal{L}$  is the Liouville operator, or Liouvillian, given by

$$\mathcal{L}\rho(t) = -i[H, \rho(t)]. \quad (2.8)$$

One can derive an exact set of equations describing the time evolution of each of the elements of the density matrix by taking the partial trace, or taking the trace over the Hilbert space  $\mathcal{H}_B$ , of the total density matrix;

$$\rho_S(t) \equiv \text{Tr}_B\{\rho(t)\}. \quad (2.9)$$

The work done by Breuer et al. [19] showed that the density matrix evolved according to the following equations.

$$\rho_{11}(t) = \rho_{11}(0)2^{-N}\text{Tr}_B\{\cos[4\sqrt{J_+J_-}\lambda t]\}, \quad (2.10)$$

$$\rho_{12}(t) = \rho_{12}(0)2^{-N}\text{Tr}_B\{\cos[2\sqrt{J_+J_-}\lambda t]\cos[2\sqrt{J_-J_+}\lambda t]\}, \quad (2.11)$$

$$\rho_{21}(t) = \rho_{21}(0)2^{-N}\text{Tr}_B\{\cos[2\sqrt{J_+J_-}\lambda t]\cos[2\sqrt{J_-J_+}\lambda t]\}. \quad (2.12)$$

From the above two equations a simplification can be made using

$$J_{\pm}|j, m\rangle = \sqrt{j(j+1) - m(m \pm 1)}|j, m \pm 1\rangle, \quad (2.13)$$

with which one can write

$$f(j, m) = \sqrt{(j+m)(j-m+1)}. \quad (2.14)$$

Using Equation (2.14) and taking the trace over the environment degrees of freedom gives the following equations:

$$\frac{\rho_{11}(t)}{\rho_{11}(0)} = \sum_{j,m} P(j, m) \cos[4f(j, m)\lambda t], \quad (2.15)$$

$$\frac{\rho_{12}(t)}{\rho_{12}(0)} = \sum_{j,m} P(j, m) \cos[2f(j, m)\lambda t] \cos[2f(j, -m)\lambda t], \quad (2.16)$$

and

$$\frac{\rho_{21}(t)}{\rho_{21}(0)} = \sum_{j,m} P(j, m) \cos[2f(j, m)\lambda t] \cos[2f(j, -m)\lambda t]. \quad (2.17)$$

In the above equations,  $P(j, m)$  is the probability for the bath to be found in a state with quantum numbers  $j$  and  $m$  [20] given by

$$P(j, m) = \frac{1}{2^N} \left[ \binom{N}{\frac{N}{2} + j} - \binom{N}{\frac{N}{2} + j + 1} \right]. \quad (2.18)$$

A plot of the probability distribution given by the above equation can be found in Figure 2.1. One may note that this probability depends on  $j$  alone. The equations (2.15), (2.16) and (2.17) represent the state of the open system, i.e. the central spin, in terms of a density matrix. Since the density matrix has the property that its trace must be unity, and the off-diagonal elements are the complex conjugate of their counterparts mirrored by the diagonal, it is sufficient to model the dynamics of the two independent density matrix elements  $\rho_{11}$  and  $\rho_{12}$ .

Figures 2.2 and 2.3 plot the two density matrix elements of interest using the

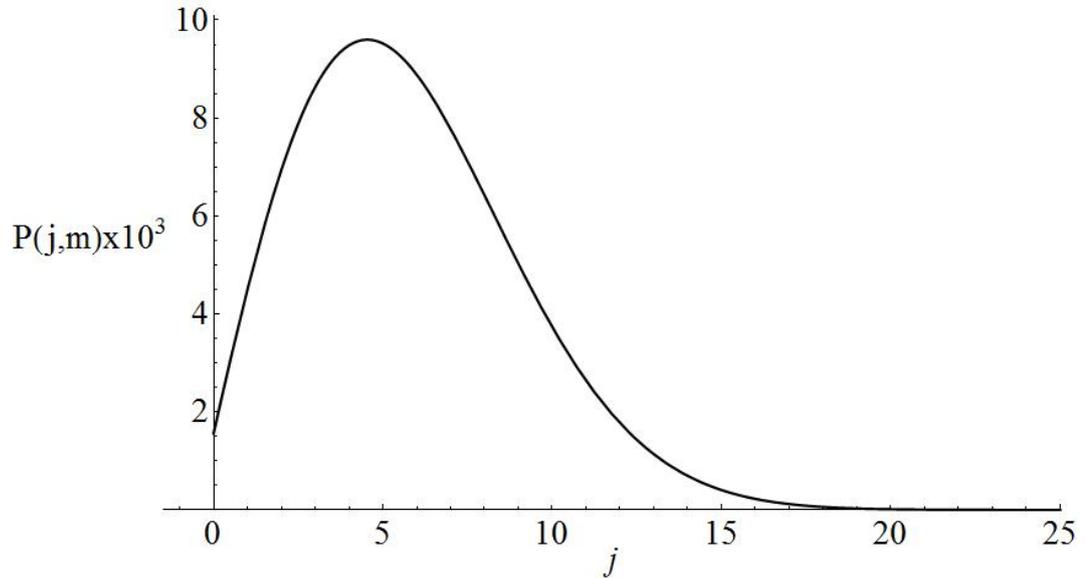


Fig. 2.1: Probability distribution of Equation (2.18); the probability of finding the bath in the state  $|j, m\rangle$ .

equations presented above. The dynamics are shown for three different cases in order to illustrate the effect of increasing the number of environment spins.

## 2.2 Non-Markovian dynamics of the spin star Model

The spin star model used in this study is both important and interesting, not only because it is an elegant example of an open quantum system, but it also not possible to treat its behaviour as a Markovian process. This means that it is not sufficient to know the state of the system at the current time in order to predict its future evolution, the history of how it evolved until this point is also necessary knowledge. It shall be demonstrated here why one cannot find a Markovian master equation for this system.

As a starting point, take the Liouville-von Neumann equation for the total system (1.15);

$$\frac{d}{dt}\rho(t) = -i[H(t), \rho(t)]. \quad (2.19)$$

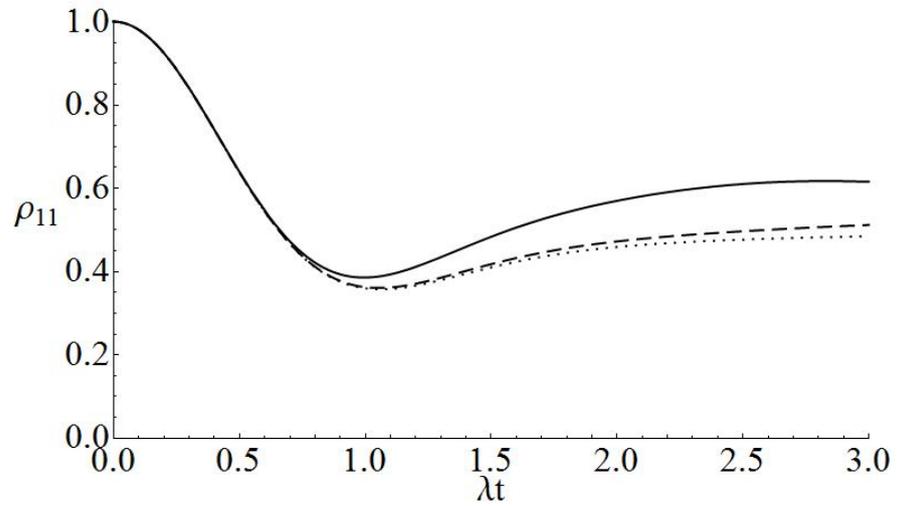


Fig. 2.2: Exact dynamics of the density matrix element  $\rho_{11}$  with the initial condition  $\rho_{11}(0) = 1$ . The number of bath spins is 20 for the solid line, 200 for the dashed line, and approaches infinity for the dotted line.

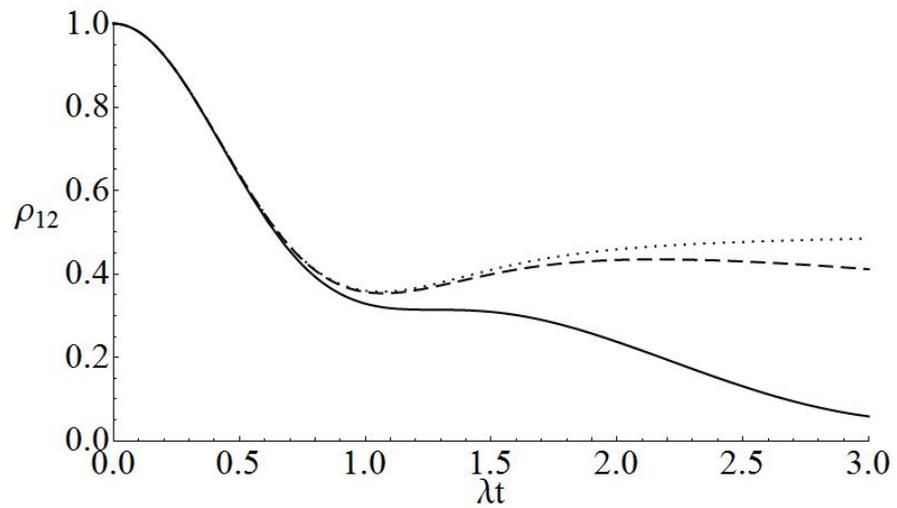


Fig. 2.3: Exact dynamics of the density matrix element  $\rho_{12}$  with the initial condition  $\rho_{12}(0) = 1$ . The number of bath spins is 20 for the solid line, 200 for the dashed line, and approaches infinity for the dotted line.

This can be written in integral form as

$$\rho(t) = \rho(0) - i \int_0^t [H(s), \rho(s)] ds. \quad (2.20)$$

If this integral form for  $\rho(t)$  is inserted back into (2.19) above, and assuming the initial condition

$$\text{Tr}_B[H(t), \rho(t)] = 0,$$

this gives

$$\frac{d}{dt}\rho(t) = - \int_0^t [H(t), [H(s), \rho(s)]] ds. \quad (2.21)$$

Now, taking the trace over the bath degrees of freedom results in the equation

$$\frac{d}{dt}\rho_S(t) = - \int_0^t \text{Tr}_B[H(t), [H(s), \rho(s)]] ds. \quad (2.22)$$

Eliminating  $\rho(t)$  from the equation above is done with the use of the Born approximation, which makes the assumption that the interaction between the central system and the bath is very weak. In other words, the bath is not affected very much over time by the central system. If the bath is very large and consists of many more particles than the central system, then this seems like a reasonable approximation. As a result of this assumption, the bath can be assumed stationary;

$$\rho_B(t) = \rho_B(0)$$

and the total system can be written as

$$\rho(t) = \rho_S(t) \otimes \rho_B(0).$$

Substituting this back into (2.22), one obtains

$$\frac{d}{dt}\rho_S(t) = - \int_0^t \text{Tr}_B[H(t), [H(s), \rho_S(s) \otimes \rho_B(0)]] ds. \quad (2.23)$$

Introducing the Bloch vector

$$v(t) = \begin{pmatrix} v_1(t) \\ v_2(t) \\ v_3(t) \end{pmatrix} = \text{Tr}_S\{\vec{\sigma}\rho_S(t)\}, \quad (2.24)$$

the master equation for the spin star model using the Born approximation can be written as

$$\frac{d}{dt}\rho_S(t) = -4\lambda^2 \int_0^t [v_+(s)\sigma_- + v_-(s)\sigma_+ + v_3(s)\sigma_z] ds, \quad (2.25)$$

where

$$v_{\pm}(t) = \frac{1}{2}(v_1(t) \pm iv_2(t)).$$

As a final step, and to arrive at a time local master equation, one replaces  $v_{\pm}(s)$  and  $v_3(s)$  with  $v_{\pm}(t)$  and  $v_3(t)$  respectively. This gives the equation, sometimes known as the Redfield equation,

$$\frac{d}{dt}\rho_S(t) = -4\lambda^2 \int_0^t [v_+(t)\sigma_- + v_-(t)\sigma_+ + v_3(t)\sigma_z] ds. \quad (2.26)$$

In order to obtain a fully Markovian time local master equation, the upper limit of the integral in the above Redfield equation is pushed to infinity. Performing all of these approximations is known as the Born-Markov approximation, and for this case of the spin star model, it can be seen that the integral above does not converge at infinity, since the integrand is non-vanishing for large  $t$ . This means that the Born-Markov approximation is not valid for this model and in order to model the decoherence effects for this system requires some other, non-Markovian, methods.



### 3. EXACT NUMERICAL SIMULATION OF THE SPIN STAR MODEL

#### 3.1 An Exact, Non-Markovian PDP Approach

The model of the open system to be studied in this chapter consists of a single spin  $\frac{1}{2}$  particle living in Hilbert space  $\mathcal{H}_S$ , embedded in a bath of identical spin  $\frac{1}{2}$  particles living in Hilbert space  $\mathcal{H}_B$ . The goal of this study is to construct a set of stochastic equations describing the evolution of this open quantum system, which may then be used in a Monte Carlo simulation. The approach presented in this chapter is a stochastic approach [21], which exactly reproduces the analytical results seen earlier.

Because of the non-Markovian dynamics inherent in the spin star model, the approach used in Section 1.3 does not work. In order to model the non-Markovian behaviour in this approach, a pair of independently evolving wavefunctions are used in constructing the density matrix.

The state vector for the total system under consideration is constructed as the product of the system and environment states,  $|\Phi(t)\rangle = |\psi(t)\rangle \otimes |\chi(t)\rangle$ . The system's state vector,  $|\psi(t)\rangle$ , lives in Hilbert space  $\mathcal{H}_S$  and the environment's state vector,  $|\chi(t)\rangle$ , lives in Hilbert space  $\mathcal{H}_B$ . The total system's state vector,  $|\Phi(t)\rangle$ , lives in the combined Hilbert space  $\mathcal{H}_S \otimes \mathcal{H}_B$ .

The density matrix for the open system can be represented as the expectation of some random operator

$$\rho(t) = E[R(t)], \quad (3.1)$$

where  $R(t) \in \mathcal{H}_S \otimes \mathcal{H}_B$  and  $R(t) = |\Phi_1(t)\rangle \langle \Phi_2(t)|$ .

Using Equation (3.1), the density matrix of the open system can be represented as the expectation  $\rho_S(t) = E[|\Phi_1(t)\rangle \langle \Phi_2(t)|]$ . This vector is constructed as a pair of independently evolving state vectors  $|\Phi_1(t)\rangle$  and  $|\Phi_2(t)\rangle$ . Each of these represent a piecewise deterministic process in which the state evolves deterministically until a random jump occurs, the state vectors instantaneously jumping into a new state, whereafter deterministic evolution continues between subsequent jumps.

As a motivation for this representation of the density matrix under consideration, one may introduce an orthonormal basis  $|\psi_i\rangle$  for the Hilbert space  $\mathcal{H}_S$  and  $|\chi_n\rangle$  for the Hilbert space  $\mathcal{H}_B$ . The density matrix  $\rho$  can then be written, with  $\rho_{ijnm} \equiv \langle \psi_i \chi_n | \rho | \psi_j \chi_m \rangle \equiv |\rho_{ijnm}| e^{2i\phi_{ijnm}}$ , as

$$\rho = \sum_{ijnm} \rho_{ijnm} |\psi_i\rangle \langle \psi_j| \otimes |\chi_n\rangle \langle \chi_m|. \quad (3.2)$$

Relabeling the indices  $ijnm$  as the collective index  $\lambda$ , one can define the states

$$|\Psi_1^\lambda\rangle = \sqrt{|\rho_\lambda|} e^{i\phi_\lambda} \psi_i \otimes \chi_n \quad (3.3)$$

and

$$|\Psi_2^\lambda\rangle = \sqrt{|\rho_\lambda|} e^{-i\phi_\lambda} \psi_j \otimes \chi_m \quad (3.4)$$

so that the density matrix can now be written as

$$\rho = \sum_{\lambda} |\Psi_1^\lambda\rangle \langle \Psi_2^\lambda|. \quad (3.5)$$

Writing  $|\Psi_\nu^\lambda\rangle = \sqrt{p_\lambda} |\Phi_\nu\rangle$  leads to the expression for the density matrix

$$\rho = \sum_{\lambda} p_\lambda |\Phi_1\rangle \langle \Phi_2| = E[|\Phi_1\rangle \langle \Phi_2|], \quad (3.6)$$

which is just the definition of the density matrix represented as the expectation of two independent state vectors which each exist with a certain probability  $p_\lambda$ .

The reduced density matrix of the open quantum system, the central spin  $\frac{1}{2}$  particle, is found by taking the partial trace over the environment's degrees of freedom of the total density matrix;  $\rho_S(t) = \text{Tr}_B[\rho(t)]$ . The density matrix for the system is then the expectation

$$\rho(t) = E[|\psi_1(t)\rangle |\chi_1(t)\rangle \langle \psi_2(t)| \langle \chi_2(t)|] \quad (3.7)$$

$$= E[|\psi_1(t)\rangle \langle \psi_2(t)| \langle \chi_2(t)| \chi_1(t)\rangle]. \quad (3.8)$$

In general, the Hamiltonian describing the interaction of the open system with

the environment, the bath of spins, is written as

$$H = \sum_{\alpha} A_{\alpha}(t) \otimes B_{\alpha}(t),$$

where  $A_{\alpha}$  and  $B_{\alpha}$  act in  $\mathcal{H}_S$  and  $\mathcal{H}_B$  respectively. With this interaction Hamiltonian the density matrix evolution can be expressed via the von Neumann equation;  $\frac{d}{dt}\rho(t) = -i[H(t), \rho(t)]$ . As previously mentioned, the states  $|\Phi_{\nu}(t)\rangle$  represent a piecewise deterministic process. The stochastic equations for this PDP shall be written here for the state vectors for the system and environment,  $|\psi_{\nu}(t)\rangle$  and  $|\chi_{\nu}(t)\rangle$ ;

$$d|\psi_{\nu}(t)\rangle = F_{\nu}dt + dJ_{\nu}, \quad (3.9)$$

and

$$d|\chi_{\nu}(t)\rangle = G_{\nu}dt + dK_{\nu}. \quad (3.10)$$

These equations describe the general dynamics of a piecewise deterministic process,  $F_{\nu}dt$  and  $G_{\nu}dt$  represent the deterministic evolution of the state vectors and  $dJ_{\nu}$  and  $dK_{\nu}$  represent the contributions from a random jump process. The jump contributions can be written as

$$dJ_{\nu} = \sum_{\alpha} (-iL_{\alpha\nu}A_{\alpha} - I)\psi_{\nu}dN_{\alpha\nu}(t) \quad (3.11)$$

and

$$dK_{\nu} = \sum_{\alpha} (M_{\alpha\nu}B_{\alpha} - I)\chi_{\nu}dN_{\alpha\nu}(t). \quad (3.12)$$

In the two equations above,  $I$  is the identity operator on the relevant Hilbert space,  $A_{\nu}$  and  $B_{\nu}$  are the operators from the interaction Hamiltonian, and  $dN_{\alpha\nu}$  are the Poisson increments. These Poisson increments are random numbers and can take on the values of 0 and 1 only. They remain zero while the state follows deterministic drift, and when  $dN_{\alpha\nu} = 1$  the state undergoes a random instantaneous jump;

$$\psi_{\nu} \rightarrow -iL_{\alpha\nu}A_{\alpha}\psi_{\nu}, \quad (3.13)$$

and

$$\chi_{\nu} \rightarrow M_{\alpha\nu}B_{\alpha}\chi_{\nu}. \quad (3.14)$$

Each  $dN_{\alpha\nu}$  behaves independently but must satisfy

$$dN_{\alpha\nu}dN_{\beta\mu} = \delta_{\alpha}^{\beta}\delta_{\nu}^{\mu}dN_{\alpha\nu} \quad (3.15)$$

so that if for any one  $\alpha$  and  $\nu$  the increment  $dN_{\alpha\nu} = 1$ , all other Poisson increments must be zero. The expectation values of these Poisson increments are

$$E[dN_{\alpha\nu}] = \Gamma_{\alpha\nu}dt, \quad (3.16)$$

where  $\Gamma_{\alpha\nu}$  is the probability per time for one jump to occur. In other words, the Poisson increment is  $dN_{\alpha\nu} = 1$  with probability  $\Gamma_{\alpha\nu}dt$ . As a consequence,  $\Gamma_{\alpha\nu}$  is the rate at which the random jump events occur.

Starting from  $R(t) = |\Phi_1(t)\rangle \langle \Phi_2(t)|$ , the random operator, one can write, using the chain rule for differentiation,

$$\begin{aligned} dR(t) &= d[|\Phi_1(t)\rangle \langle \Phi_2(t)|] \\ &= [d|\Phi_1(t)\rangle] \langle \Phi_2(t)| + |\Phi_1(t)\rangle [d\langle \Phi_2(t)|] + [d|\Phi_1(t)\rangle][d\langle \Phi_2(t)|] \\ &= [d|\Phi_1(t)\rangle] \langle \Phi_2(t)| + |\Phi_1(t)\rangle [d\langle \Phi_2(t)|] \end{aligned} \quad (3.17)$$

The third term in the second line in the above set of equations vanishes since it involves the term  $dN_{\alpha_1}dN_{\beta_2}$  which is equal to zero always. Using the definition  $|\Phi_{\nu}(t)\rangle = |\psi_{\nu}(t)\rangle \otimes |\chi_{\nu}(t)\rangle$ , one obtains

$$d|\Phi_{\nu}(t)\rangle = d|\psi_{\nu}(t)\rangle \otimes |\chi_{\nu}(t)\rangle + |\psi_{\nu}(t)\rangle \otimes d|\chi_{\nu}(t)\rangle + d|\psi_{\nu}(t)\rangle \otimes d|\chi_{\nu}(t)\rangle. \quad (3.18)$$

Using the form previously shown for the differential form of the state vectors for the open system and the environment, (3.9) and (3.10), the above equation becomes

$$\begin{aligned} d|\Phi_{\nu}(t)\rangle &= (F_{\nu}dt + dJ_{\nu}) \otimes |\chi_{\nu}(t)\rangle \\ &\quad + |\psi_{\nu}(t)\rangle \otimes (G_{\nu}dt + dK_{\nu}) \\ &\quad + (F_{\nu} \otimes G_{\nu})dt^2 + (dJ_{\nu} \otimes G_{\nu} + F_{\nu} \otimes dK_{\nu})dt \\ &\quad + dJ_{\nu} \otimes dK_{\nu}. \end{aligned} \quad (3.19)$$

Both terms in the third line of the above equation are of the order  $dt^2$ , and

subsequently vanish. Substituting in the definitions for  $dJ_\nu$  and  $dK_\nu$ , (3.11) and (3.12), the last term in (3.19) can be written as

$$\begin{aligned} dJ_\nu \otimes dK_\nu &= \sum_{\alpha} [(-iL_{\alpha\nu}A_\alpha - I)\psi_\nu \otimes (M_{\alpha\nu}B_\alpha - I)\chi_\nu] dN_{\alpha\nu} \\ &= -dJ_\nu \otimes \chi_\nu \\ &\quad + \sum_{\alpha} [(-iL_{\alpha\nu}A_\alpha - I)\psi_\nu \otimes M_{\alpha\nu}B_\alpha\chi_\nu] dN_{\alpha\nu}. \end{aligned} \quad (3.20)$$

Finally, substituting the above equation back into (3.19), one arrives at

$$\begin{aligned} d|\Phi_\nu(t)\rangle &= F_\nu dt \otimes \chi_\nu + \psi_\nu \otimes G_\nu dt \\ &\quad + \sum_{\alpha} -iL_{\alpha\nu}A_\alpha\psi_\nu \otimes M_{\alpha\nu}B_\alpha\chi_\nu dN_{\alpha\nu} \\ &\quad + \psi_\nu \otimes \sum_{\alpha} (M_{\alpha\nu}B_\alpha - I)\chi_\nu dN_{\alpha\nu} \\ &\quad - \sum_{\alpha} \psi_\nu \otimes M_{\alpha\nu}B_\alpha\chi_\nu dN_{\alpha\nu} \\ &= F_\nu dt \otimes \chi_\nu + \psi_\nu \otimes (G_\nu dt - \sum_{\alpha} dN_{\alpha\nu}\chi_\nu) \\ &\quad + \sum_{\alpha} -iL_{\alpha\nu}A_\alpha\psi_\nu \otimes M_{\alpha\nu}B_\alpha\chi_\nu dN_{\alpha\nu}. \end{aligned} \quad (3.21)$$

The above equation describes the time evolution of the stochastic state vector  $|\Phi_\nu(t)\rangle$  as a result of both deterministic drift evolution and the random jump processes. In order for the first two terms to vanish when taking the average over all the Poisson increments,

$$G_\nu = \sum_{\alpha} \Gamma_{\alpha\nu}\chi_\nu = \Gamma_\nu\chi_\nu$$

and

$$F_\nu = 0.$$

The complex valued functionals  $L_{\alpha\nu}$  and  $M_{\alpha\nu}$  are defined as  $\frac{1}{L_{\alpha\nu}M_{\alpha\nu}} = \Gamma_{\alpha\nu}$ . Combining these definitions with (3.21) leads to the following expression for the differential

evolution of the stochastic states  $|\Phi_\nu(t)\rangle$ ;

$$\begin{aligned} d|\Phi_\nu(t)\rangle &= \psi_\nu \otimes (\Gamma_\nu dt - \sum_\alpha dN_{\alpha\nu})\chi_\nu \\ &\quad - i \sum_\alpha \Gamma_{\alpha\nu}^{-1} (A_\alpha \psi_\nu) \otimes (B_\alpha \chi_\nu) dN_{\alpha\nu}. \end{aligned} \quad (3.22)$$

In order for the jump processes to conserve the norm of the stochastic state vectors,  $L_{\alpha\nu}$  and  $M_{\alpha\nu}$  are chosen such that

$$L_{\alpha\nu} = \frac{\|\psi_\nu(t)\|}{\|A_\alpha \psi_\nu(t)\|} \quad (3.23)$$

and

$$M_{\alpha\nu} = \frac{\|\chi_\nu(t)\|}{\|B_\alpha \chi_\nu(t)\|}, \quad (3.24)$$

and consequently the jump rate  $\Gamma_{\alpha\nu}$  is defined as

$$\Gamma_{\alpha\nu} = \frac{\|A_\alpha \psi_\nu(t)\| \cdot \|B_\alpha \chi_\nu(t)\|}{\|\psi_\nu(t)\| \cdot \|\chi_\nu(t)\|}. \quad (3.25)$$

Finally, the differential equations for this process for each of the system and environment states respectively are

$$d|\psi_\nu(t)\rangle = \sum_\alpha \left( -i \frac{\|\psi_\nu(t)\|}{\|A_\alpha \psi_\nu(t)\|} A_\alpha - I \right) \psi_\nu dN_{\alpha\nu}(t), \quad (3.26)$$

and

$$d|\chi_\nu(t)\rangle = \Gamma_\nu \chi_\nu dt + \sum_\alpha \left( \frac{\|\chi_\nu(t)\|}{\|B_\alpha \chi_\nu(t)\|} B_\alpha - I \right) \chi_\nu dN_{\alpha\nu}(t). \quad (3.27)$$

It can be seen from the above equations that  $|\psi_\nu(t)\rangle$  is a norm conserving jump process and  $|\chi_\nu(t)\rangle$  is a jump process with linear drift whose norm increases exponentially. As a result of this exponential increase of the norm, this stochastic PDP is good for simulations where the time period is short, since the processing time also increases exponentially with the simulation time. An appropriate time scale for which this simulation is efficient is given by

$$t_f = \frac{1}{2} \Gamma_{max}$$

where  $\Gamma_{max} \leq \Gamma_\nu$  for any  $\nu$ , giving an upper bound for the jump rates.

The equations above, (3.26) and (3.27), describe the dynamics of the jump processes of the system and the environment respectively. It has been shown that using these equations, a model can be simulated which exhibits the non-Markovian behaviour of the spin star system.

### 3.2 The PDP for the spin star Model

In this section, the aim is to apply the general approach of the previous section to the spin star model presented in Chapter 2. The model to be simulated consists of a bath of  $N$  spin one-half particles surrounding a central spin [22]. This model is illustrated by Figure 3.1, a “quantum spinning top” surrounded by an environment of identical spins. This figure illustrates the symmetry of the model, geometrically and with respect to the coupling strength between each environment spin with the central system. This bath exists initially in the state  $|j, m\rangle$ , where  $j$  is the total collective spin and  $m$  is the  $z$ -component of the total spin. The probability for this bath of  $N$  spins to exist in state  $|j, m\rangle$  is given, as in (2.18), by

$$P(j, m) = \frac{1}{2^N} \left[ \binom{N}{\frac{N}{2} + j} - \binom{N}{\frac{N}{2} + j + 1} \right]. \quad (3.28)$$

As a reminder, from the first chapter, the Hamiltonian of this system is given by

$$H = \frac{\lambda}{\sqrt{N}} (\sigma_+ J_- + \sigma_- J_+). \quad (3.29)$$

The initial condition of the system is the state

$$|\Phi(0)\rangle = |S, S_z\rangle \otimes |j, m\rangle. \quad (3.30)$$

Writing the Hamiltonian (3.29) in the form

$$H = \sum_{\alpha} A_{\alpha} \otimes B_{\alpha},$$

where  $A \in \mathcal{H}_s$  and  $B \in \mathcal{H}_B$ , leads to the following equations describing the jump

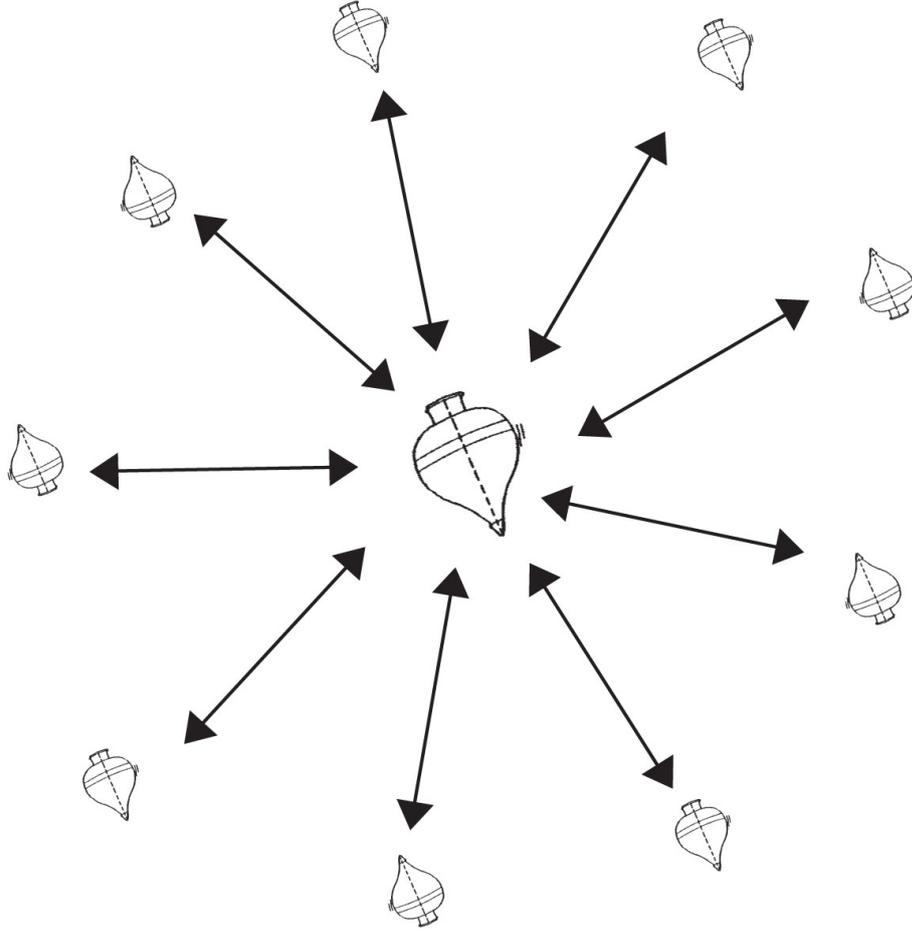


Fig. 3.1: A diagram representing the spin star model, a central spin half particle interacting with a bath of spins.

processes for the central spin and bath states;

$$\begin{aligned}
 |S, S_z\rangle &\rightarrow \frac{-i\| |S, S_z\rangle \|}{\| \sigma_{\pm} |S, S_z\rangle \|} \sigma_{\pm} |S, S_z\rangle \\
 |j, m\rangle &\rightarrow \frac{\| |j, m\rangle \|}{\| J_{\mp} |j, m\rangle \|} J_{\mp} |j, m\rangle.
 \end{aligned} \tag{3.31}$$

This model describes a two level system having two distinct jump rates;  $|\frac{1}{2}, -\frac{1}{2}\rangle \rightarrow |\frac{1}{2}, \frac{1}{2}\rangle$  and  $|\frac{1}{2}, \frac{1}{2}\rangle \rightarrow |\frac{1}{2}, -\frac{1}{2}\rangle$ . The jump rates for this process can be calculated, as in

(3.25), using

$$\Gamma_{\alpha\nu} = \frac{\|A_\alpha\psi_\nu\| \cdot \|B_\alpha\chi_\nu\|}{\|\psi_\nu\| \cdot \|\chi_\nu\|}.$$

The system will randomly jump between states  $|\frac{1}{2}, -\frac{1}{2}\rangle$  and  $|\frac{1}{2}, \frac{1}{2}\rangle$ , with each jump contributing a factor  $(-i)$ . Additionally, if the system makes an even number of jumps after initially starting in a given state, it will with certainty end in the same state. If, however, the system makes an odd number of jumps after starting in a given state, it will certainly end up in the other state.

Explicitly, if the system starts in the state  $|\frac{1}{2}, -\frac{1}{2}\rangle$ , then after an even number of jumps

$$\begin{aligned} |S, S_z\rangle &= (-i)^{n_j} |\frac{1}{2}, -\frac{1}{2}\rangle \\ |j, m\rangle &= |j, m\rangle e^{\Gamma(j,m)t}, \end{aligned} \tag{3.32}$$

where  $n_j$  is the number of jumps that have occurred, or after an odd number of jumps

$$\begin{aligned} |S, S_z\rangle &= (-i)^{n_j} |\frac{1}{2}, \frac{1}{2}\rangle, \\ |j, m\rangle &= |j, m-1\rangle e^{\Gamma(j,m)t}. \end{aligned} \tag{3.33}$$

The jump rates for each of the two possible jumps,  $\Gamma_{up}(j, m)$  and  $\Gamma_{down}(j, m)$ , are now calculated according to (3.25).

$$\begin{aligned}
\Gamma_{up}(j, m) &= \frac{\lambda}{\sqrt{N}} \frac{\|\sigma_+ |\frac{1}{2}, -\frac{1}{2}\rangle\| \cdot \|J_- |j, m\rangle\|}{\| |\frac{1}{2}, -\frac{1}{2}\rangle\| \cdot \| |j, m\rangle\|} \\
&= \frac{\lambda}{\sqrt{N}} \frac{\|[\frac{1}{2}(\frac{1}{2} + 1) + \frac{1}{2}(-\frac{1}{2} + 1)]^{\frac{1}{2}} |\frac{1}{2}, \frac{1}{2}\rangle\| \cdot \|J_- |j, m\rangle\|}{\| |\frac{1}{2}, -\frac{1}{2}\rangle\| \cdot \| |j, m\rangle\|} \\
&= \frac{\lambda}{\sqrt{N}} \frac{\| |\frac{1}{2}, \frac{1}{2}\rangle\| \cdot \|J_- |j, m\rangle\|}{\| |\frac{1}{2}, -\frac{1}{2}\rangle\| \cdot \| |j, m\rangle\|} \\
&= \frac{\lambda}{\sqrt{N}} \|J_- |j, m\rangle\| \\
&= \frac{\lambda}{\sqrt{N}} \|[j(j+1) - (m-1)m]^{\frac{1}{2}} |j, m-1\rangle\| \\
&= \frac{\lambda}{\sqrt{N}} [j(j+1) - (m-1)m]^{\frac{1}{2}}. \tag{3.34}
\end{aligned}$$

In exactly the same way the remaining jump rate is calculated as

$$\begin{aligned}
\Gamma_{down}(j, m) &= \frac{\lambda}{\sqrt{N}} \frac{\|\sigma_- |\frac{1}{2}, \frac{1}{2}\rangle\| \cdot \|J_+ |j, m-1\rangle\|}{\| |\frac{1}{2}, \frac{1}{2}\rangle\| \cdot \| |j, m-1\rangle\|} \\
&= \frac{\lambda}{\sqrt{N}} \frac{\|[\frac{1}{2}(\frac{1}{2} + 1) - \frac{1}{2}(\frac{1}{2} - 1)]^{\frac{1}{2}} |\frac{1}{2}, -\frac{1}{2}\rangle\| \cdot \|J_+ |j, m-1\rangle\|}{\| |\frac{1}{2}, \frac{1}{2}\rangle\| \cdot \| |j, m-1\rangle\|} \\
&= \frac{\lambda}{\sqrt{N}} \frac{\| |\frac{1}{2}, -\frac{1}{2}\rangle\| \cdot \|J_+ |j, m-1\rangle\|}{\| |\frac{1}{2}, \frac{1}{2}\rangle\| \cdot \| |j, m-1\rangle\|} \\
&= \frac{\lambda}{\sqrt{N}} \|J_+ |j, m-1\rangle\| \\
&= \frac{\lambda}{\sqrt{N}} \|[j(j+1) - (m-1)m]^{\frac{1}{2}} |j, m\rangle\| \\
&= \frac{\lambda}{\sqrt{N}} [j(j+1) - (m-1)m]^{\frac{1}{2}}. \tag{3.35}
\end{aligned}$$

It is important to note that the jump rate may depend not only on the bath state  $|j, m\rangle$ , but also on the state of the central spin. The total jump rate  $\Gamma(j, m)$  is the sum of all allowed jump rates,

$$\Gamma(j, m) = \sum_{\alpha} \Gamma_{\alpha}(j, m).$$

Whether or not a particular jump is allowed is dependant on the state of the central spin. In this particular case, this model of a two level system has a total of two jumps and at any one time, only one of them are allowed. Additionally, one notices that these jump rates for the two jumps are equal.

Having calculated the jump rates, and using (3.3) and (3.4) along with the definition for the density matrix in the form of an expectation (3.1), the element of the density matrix of the central spins  $\rho_{11}$  can be expressed as

$$\begin{aligned}
 \rho_{11}(t) &= \langle \frac{1}{2}, -\frac{1}{2} | \rho_S(t) | \frac{1}{2}, -\frac{1}{2} \rangle \\
 &= E[\langle \frac{1}{2}, -\frac{1}{2} | \psi_1(t) \rangle \langle \psi_2(t) | \frac{1}{2}, -\frac{1}{2} \rangle \langle \chi_2(t) | \chi_1(t) \rangle] \\
 &= E[W(n_{j_1}, n_{j_2}) (-i)^{n_{j_1}} (+i)^{n_{j_2}} e^{\Gamma(j,m)t} e^{\Gamma(j,m)t}] \\
 &= E[W(n_{j_1}, n_{j_2}) (-1)^{\frac{n_{j_1}+n_{j_2}}{2}} e^{2\Gamma(j,m)t}]. \tag{3.36}
 \end{aligned}$$

In the above equation,  $W(n_{j_1}, n_{j_2})$  is a function which is 1 if both it's arguments are even, and 0 otherwise. The values  $n_{j_1}$  and  $n_{j_2}$  represent the number of jumps the states  $|\psi_1(t)\rangle$  and  $|\psi_2(t)\rangle$  have undergone respectively. It is also assumed that the initial condition of the system is such that the central spin begins in state  $|\psi(0)\rangle = |\frac{1}{2}, -\frac{1}{2}\rangle$ . It is under this assumption that the density matrix element to be considered can only be non-zero if the number of jumps that each of the two states  $|\psi_\nu(t)\rangle$  is even.

### 3.3 The Numerical Algorithm

This section describes in detail the construction of the algorithm used to simulate the trajectory followed by the density matrix of the central spin's state [22]. The first part of the algorithm involves setting up parameters such as the number of bath spins, the final time until which the simulation will run, and the coupling constant. Additionally, this parameter setup phase is where the probability distribution function for states  $|j, m\rangle$  is set up. Utilising the properties of the logarithm function provides a significant speedup since the factorials in (2.18) can be replaced with sums. A cumulative probability distribution function is set up for all possible  $j$  values running from 1 to half the number of bath spins,  $\frac{N}{2}$ . It can be seen that for this case, the probability of the bath existing in state  $|j, m\rangle$ , that the probability distribution, given by (2.18), is dependant on  $j$  but not on  $m$ . As a result, the quantum number  $j$  is

picked according to this probability but the corresponding quantum number  $m$  is chosen according to a uniform distribution. This is done because each  $m$  is equally likely for any given value of  $j$ .

Once the parameters are set up, the two independently evolving states  $|\psi_1(t)\rangle$  and  $|\psi_2(t)\rangle$  are simulated. One realisation of this simulation involves stepping through time from  $t = 0$  until the final time  $t = t_f$  in steps of the random waiting time  $\tau = \frac{-\log(\eta)}{\Gamma}$  where  $\eta$  is a uniformly distributed number between 0 and 1, and as a result the jumps constitute a Poisson process. Every time a new  $\tau$  is found and added to the existing time, this indicates that a jump occurs. Ensuring that the time does not run past  $t_f$ , a record is kept of when these jumps occur and to which new state the system has jumped. In this case, the system exists in either  $|\frac{1}{2}, -\frac{1}{2}\rangle$  or  $|\frac{1}{2}, \frac{1}{2}\rangle$  and so this is trivial since there is only one possible state to jump into. However, if a different system is modeled it may be the case that the state jumps into multiple possible other states with the probability of jumping into the  $r$ 'th state given by

$$P_j(r) = \sum_r \Gamma_r(j, m). \quad (3.37)$$

As well as recording which state is occupied at each time interval, a record must also be kept of what factors the jumps have contributed to the state's evolution. Recall that every jump contributes a factor  $(-i)$  to  $|\psi\rangle$  and between jumps there is no drift. For  $|\chi\rangle$ , the deterministic drift is the factor  $e^{\Gamma t}$ , but care must be taken since  $\Gamma(j, m)$  may be dependant on the currently occupied state.

Once this procedure has been concluded twice, once for each independently evolving  $|\Phi_\nu(t)\rangle$ , this constitutes one realisation. For each realisation, a new pair of quantum numbers  $j$  and  $m$  are picked for the bath state, and then for this bath state the composite system state is simulated twice, once for each of the two independent  $|\Phi_\nu(t)\rangle$ 's.

If the initial condition is assumed to be  $|\frac{1}{2}, -\frac{1}{2}\rangle$ , the density matrix element  $\rho_{11}(t)$  for a specified time interval can be calculated by averaging over many realisations of the product

$$\langle \frac{1}{2}, -\frac{1}{2} | \psi_1(t) \rangle \langle \psi_2(t) | \frac{1}{2}, -\frac{1}{2} \rangle \langle \chi_2(t) | \chi_1(t) \rangle, \quad (3.38)$$

where  $\langle \frac{1}{2}, -\frac{1}{2} | \psi_1(t) \rangle$  is either 0 or  $(-i)^{n_{j1}}$ , where  $n_{j1}$  is the number of jumps  $|\psi_1(t)\rangle$

has undergone. Similarly,  $\langle \psi_2(t) | \frac{1}{2}, -\frac{1}{2} \rangle$  is either 0 or  $(+i)^{n_{j_2}}$ , where  $n_{j_2}$  is the number of jumps  $|\psi_2(t)\rangle$  has undergone. The contributions from  $\langle \chi_2(t) | \chi_1(t) \rangle$  are each just  $e^{\Gamma t}$  but as previously mentioned, one must be careful to remember that  $\Gamma(j, m)$  may depend on which state  $\psi(t)$  is in at that time. If the model demands it, one may use the record of which states were occupied at each time interval to construct the function  $\Gamma$  for each time interval. Averaging the product of (3.38) with the probability distribution (2.18) over many realisations is effectively taking the trace over the bath degrees of freedom, or in other words calculating the expectation of the product above. The result is an approximation of the density matrix element's trajectory which approaches the exact value given enough realisations.

### 3.4 Results

The simulation algorithm described in the previous section was run using  $10^6$  realisations and again with  $10^7$  realisations to give some idea as to the tradeoff between accuracy and computing cost. It can be clearly seen that in the interval  $\lambda t \in [0, 1]$  the results of the simulation converge well to the exact solution with a reasonable cost of computing time.

In the construction of the algorithm for simulating the dynamics of this model, it was shown that for each of the two independently evolving states, one component did not grow in magnitude and just included a term of the form  $(i)^n$  while the other, the bath's component, grew exponentially as a term of the form  $\exp(\Gamma t)$ . It is clear that this second component will grow exponentially if the exponent is greater than one, which is usually the case as  $\lambda t$  runs past one. This algorithm is designed in such a way that as the number of realisations approaches infinity, the expectation of this exponential term approaches one. This means that whilst an increase in  $\lambda t$  will introduce greater errors, this can be offset by increasing the number of realisations used in computing the expectation to the point that the numerical plots approach the analytical solution exactly as the number of realisations increase. This tradeoff between computation time and accuracy is exponential, this means that this algorithm used in this study is reasonable to use for the region  $0 \leq \lambda t \leq 1$  and as is evident in the figures, errors soon play a dominant role thereafter. For each of the plots the time was run from  $\lambda t$  between zero and one, and was run for both  $10^6$  and  $10^7$  realisations to illustrate the error reduction when more realisations are used.

From these results it can be seen that using the algorithm above is very efficient

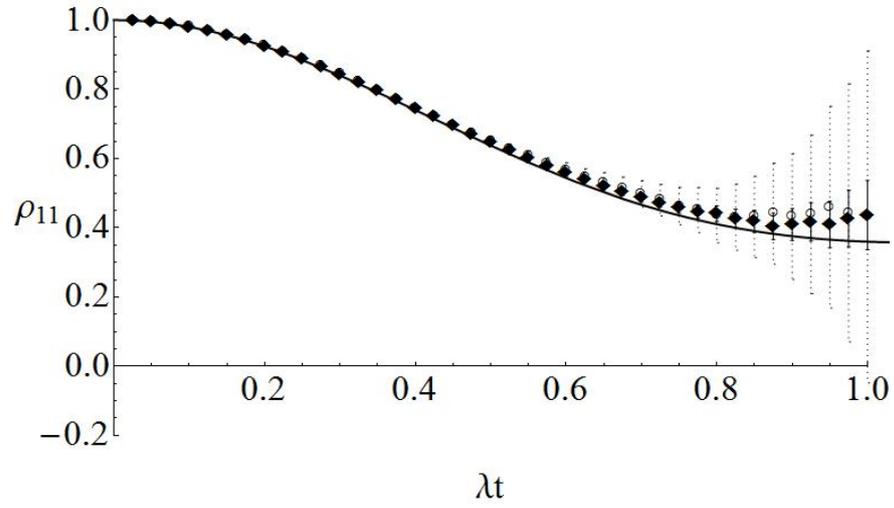


Fig. 3.2: Numerical plot of density matrix element  $\rho_{11}$  where the circles represent  $10^6$  realisations and the diamonds  $10^7$  realisations with the initial condition  $|\psi(0)\rangle = |\frac{1}{2}, -\frac{1}{2}\rangle$ . The analytical solution is represented by the solid line.

if the behaviour one wishes to model lies within the aforementioned bounds and approaches the exact solution. Additionally, the algorithm presented here is designed to calculate the dynamics of every density matrix element resulting in a complete statistical description of the open system.

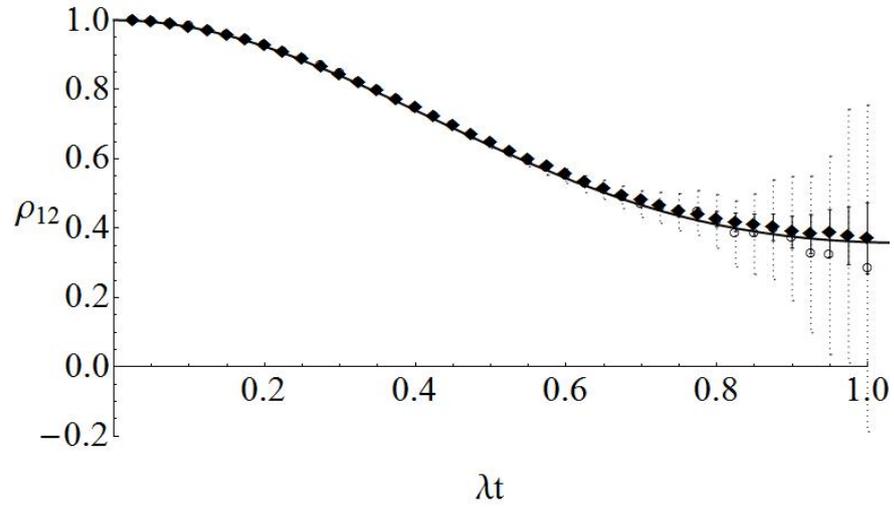


Fig. 3.3: Numerical plot of density matrix element  $\rho_{12}$  where the circles represent  $10^6$  realisations and the diamonds  $10^7$  realisations with the initial condition  $|\psi(0)\rangle = \frac{1}{2}(|\frac{1}{2}, \frac{1}{2}\rangle + |\frac{1}{2}, -\frac{1}{2}\rangle)$ . The analytical solution is represented by the solid line.

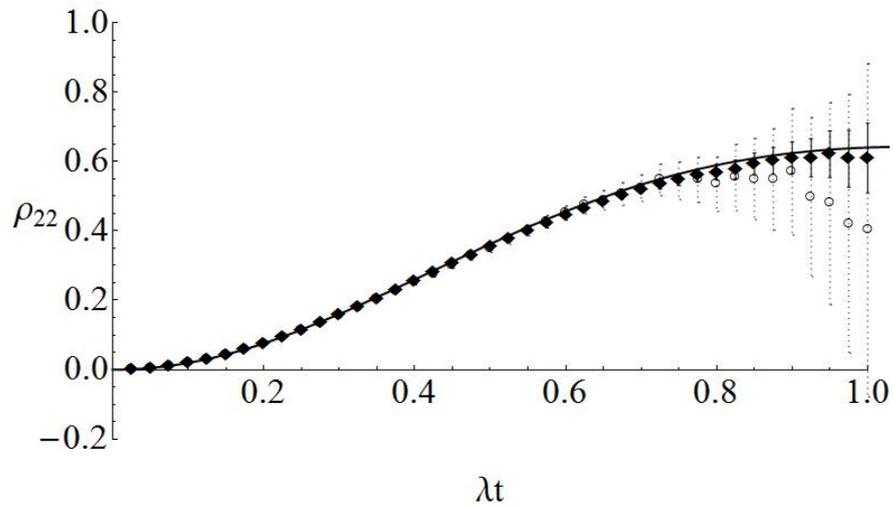


Fig. 3.4: Numerical plot of density matrix element  $\rho_{22}$  where the circles represent  $10^6$  realisations and the diamonds  $10^7$  realisations with the initial condition  $|\psi(0)\rangle = |\frac{1}{2}, -\frac{1}{2}\rangle$ . The analytical solution is represented by the solid line.



## 4. SUBSTITUTING A SPIN 1 QUTRIT FOR THE CENTRAL SPIN

### 4.1 PDP for Spin 1 case

Instead of a single spin one-half particle as the central system, the case where the central system consists of a single spin one particle surrounded by  $N$  spin one-half particles is investigated. This model is illustrated by Figure 4.1, the most notable change from the previous chapter is the central spin. In this model, the central spin exists as a three level system. In contrast to the two level system of a spin half particle, a spin one particle can be treated as a three level system with probabilities for transition between these three states which shall be explored. The bath is unchanged from the previous chapter and retains the symmetry that enables this model to be solved analytically. Nevertheless, it is interesting to study the numerical techniques presented in this study and compare their results to the analytical results given in [23].

The bath exists initially in the state  $|j, m\rangle$ , where  $j$  is the total collective spin and  $m$  is the  $z$ -component of the total spin. The probability for the bath to exist in state  $|j, m\rangle$  is given again, as in (2.18), by

$$P(j, m) = \frac{1}{2^N} \left[ \binom{N}{\frac{N}{2} + j} - \binom{N}{\frac{N}{2} + j + 1} \right]. \quad (4.1)$$

The Hamiltonian of this system is given by

$$H = \frac{\lambda}{\sqrt{N}} (\sigma_+ J_- + \sigma_- J_+). \quad (4.2)$$

The initial condition of the system is the state

$$|\Phi(0)\rangle = |S, S_z\rangle \otimes |j, m\rangle. \quad (4.3)$$

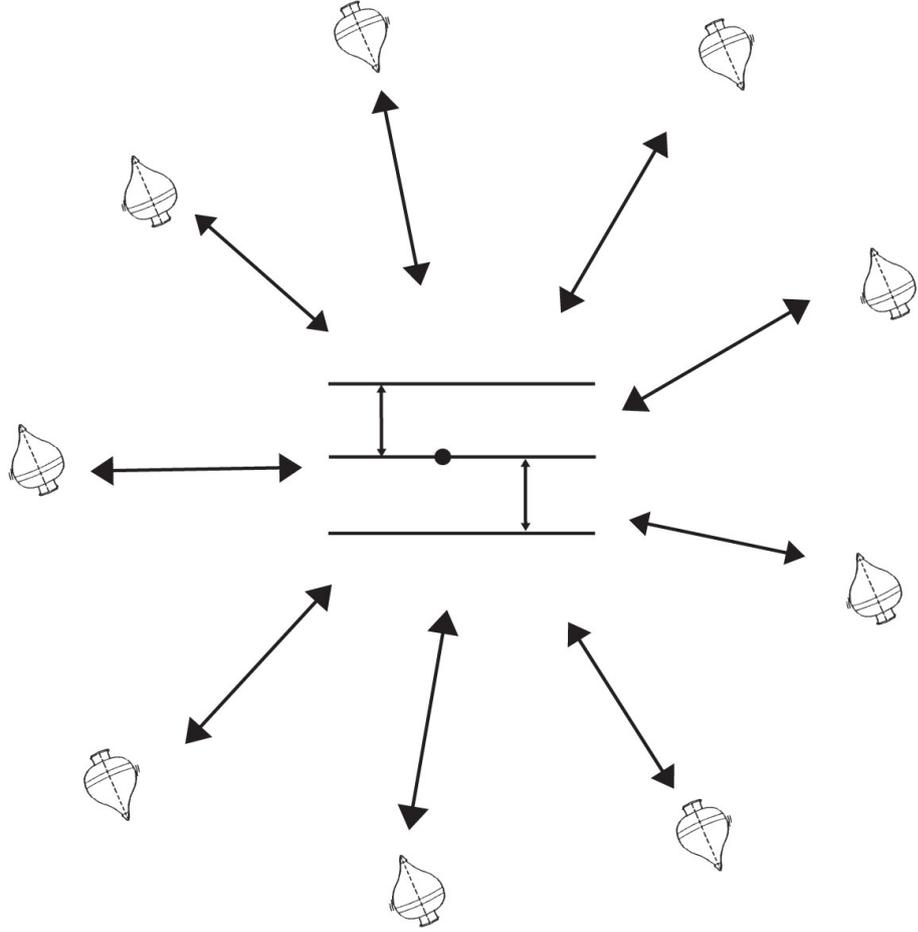


Fig. 4.1: A diagram representing a spin star model where the central system is a three level system, or qutrit, interacting with a bath of spin half particles.

Writing the Hamiltonian (4.2) in the form

$$H = \sum_{\alpha} A_{\alpha} \otimes B_{\alpha},$$

where  $A \in \mathcal{H}_s$  and  $B \in \mathcal{H}_B$ , leads to the following equations describing the jump

processes for the central spin and bath states;

$$\begin{aligned} |S, S_z\rangle &\rightarrow \frac{-i\| |S, S_z\rangle \|}{\| \sigma_{\pm} |S, S_z\rangle \|} \sigma_{\pm} |S, S_z\rangle \\ |j, m\rangle &\rightarrow \frac{\| |j, m\rangle \|}{\| J_{\mp} |j, m\rangle \|} J_{\mp} |j, m\rangle. \end{aligned} \quad (4.4)$$

In contrast to the previous chapter, this model describes a three level system having four distinct jumps;  $|1, -1\rangle \rightarrow |1, 0\rangle$ ,  $|1, 0\rangle \rightarrow |1, -1\rangle$ ,  $|1, 1\rangle \rightarrow |1, 0\rangle$  and  $|1, 0\rangle \rightarrow |1, 1\rangle$ . The jump rates for this process can again be calculated according to (3.25), using

$$\Gamma_{\alpha\nu} = \frac{\| A_{\alpha}\psi_{\nu} \| \cdot \| B_{\alpha}\chi_{\nu} \|}{\| \psi_{\nu} \| \cdot \| \chi_{\nu} \|}.$$

This system will randomly jump between the three states  $|1, -1\rangle$ ,  $|1, 0\rangle$  and  $|1, 1\rangle$ , with each jump contributing a factor  $(-i)$ . Complications arise from the fact that an even number of jumps no longer guarantees with certainty the final state and it should also be observed that the four jump rates are not equal unlike in the previous chapter. If the system makes an even number of jumps after initially starting in the state  $|1, 0\rangle$ , it will with certainty end in the same state. If, however, the system makes an odd number of jumps from the initial state  $|1, 0\rangle$ , it will end up in one of the two remaining states with a some probability. Similarly, if the system starts in either of the states  $|1, -1\rangle$  or  $|1, 1\rangle$ , an odd number of jumps will result in the final state  $|1, 0\rangle$  with absolute certainty. On the other hand, an even number of jumps from the initial states  $|1, -1\rangle$  or  $|1, 1\rangle$  will result in the final state being either  $|1, -1\rangle$  or  $|1, 1\rangle$  with the same aforementioned probability. This probability is given by the two jump rates out of the state  $|1, 0\rangle$ . The probability to jump from  $|1, 0\rangle$  to  $|1, 1\rangle$  is given by the equation

$$\pi_{0\rightarrow 1} = \frac{\Gamma_{0\rightarrow 1}}{\Gamma_{0\rightarrow 1} + \Gamma_{0\rightarrow -1}}, \quad (4.5)$$

where  $\Gamma_{0\rightarrow 1}$  and  $\Gamma_{0\rightarrow -1}$  represent the probabilities of jumping from  $|1, 0\rangle$  to  $|1, 1\rangle$  and  $|1, 0\rangle$  to  $|1, -1\rangle$  respectively. In the same way, the probability to jump from  $|1, 0\rangle$  to  $|1, -1\rangle$  is given by the equation

$$\pi_{0\rightarrow -1} = \frac{\Gamma_{0\rightarrow -1}}{\Gamma_{0\rightarrow 1} + \Gamma_{0\rightarrow -1}}. \quad (4.6)$$

More explicitly, if the system starts in state  $|1, 1\rangle$ , then after an even number of

jumps

$$\begin{aligned} |S, S_z\rangle &= (-i)^{n_j} |1, 1\rangle \\ |j, m\rangle &= |j, m\rangle \exp\left(\sum_i^{n_j} \Gamma_i(j, m)t_i\right), \end{aligned} \quad (4.7)$$

with probability  $\pi_{0\rightarrow 1}$ , or

$$\begin{aligned} |S, S_z\rangle &= (-i)^{n_j} |1, -1\rangle \\ |j, m\rangle &= |j, m+2\rangle \exp\left(\sum_i^{n_j} \Gamma_i(j, m)t_i\right), \end{aligned} \quad (4.8)$$

with probability  $\pi_{0\rightarrow -1}$  where  $n_j$  is the number of jumps that have occurred,  $\Gamma_i$  is the jump rate after  $i$  jumps and  $t_i$  is the random waiting time before the  $i$ th jump. This is an important change to the previous chapter since the jump rate is no longer constant but rather depends on the state of the system at a given time. After an odd number of jumps

$$\begin{aligned} |S, S_z\rangle &= (-i)^{n_j} |1, 0\rangle \\ |j, m\rangle &= |j, m+1\rangle \exp\left(\sum_i^{n_j} \Gamma_i(j, m)t_i\right). \end{aligned} \quad (4.9)$$

The jump rates for each of the four possible jumps,  $\Gamma_{-1\rightarrow 0}(j, m)$ ,  $\Gamma_{1\rightarrow 0}(j, m)$ ,  $\Gamma_{0\rightarrow -1}(j, m)$  and  $\Gamma_{0\rightarrow 1}(j, m)$ , are now calculated according to (3.25).

$$\begin{aligned}
\Gamma_{-1 \rightarrow 0}(j, m) &= \frac{\lambda}{\sqrt{N}} \frac{\|\sigma_+ |1, -1\rangle\| \cdot \|J_- |j, m\rangle\|}{\| |1, -1\rangle\| \cdot \| |j, m\rangle\|} \\
&= \frac{\lambda}{\sqrt{N}} \frac{\|[\frac{1}{2}(1(1+1) + 1(-1+1))]^{\frac{1}{2}} |1, 0\rangle\| \cdot \|J_- |j, m\rangle\|}{\| |1, -1\rangle\| \cdot \| |j, m\rangle\|} \\
&= \frac{\lambda}{\sqrt{N}} \frac{\| |1, 0\rangle\| \cdot \|J_- |j, m\rangle\|}{\| |1, -1\rangle\| \cdot \| |j, m\rangle\|} \\
&= \frac{\lambda}{\sqrt{N}} \|J_- |j, m\rangle\| \\
&= \frac{\lambda}{\sqrt{N}} \| [j(j+1) - (m-1)m]^{\frac{1}{2}} |j, m-1\rangle \| \\
&= \frac{\lambda}{\sqrt{N}} [j(j+1) - (m-1)m]^{\frac{1}{2}}. \tag{4.10}
\end{aligned}$$

In exactly the same way the remaining jump rates are calculated as

$$\begin{aligned}
\Gamma_{0 \rightarrow 1}(j, m) &= \frac{\lambda}{\sqrt{N}} \frac{\|\sigma_+ |1, 0\rangle\| \cdot \|J_- |j, m-1\rangle\|}{\| |1, 0\rangle\| \cdot \| |j, m-1\rangle\|} \\
&= \frac{\lambda}{\sqrt{N}} \frac{\|[\frac{1}{2}(1(1+1) + 0(0+1))]^{\frac{1}{2}} |1, 1\rangle\| \cdot \|J_- |j, m-1\rangle\|}{\| |1, 0\rangle\| \cdot \| |j, m-1\rangle\|} \\
&= \frac{\lambda}{\sqrt{N}} \frac{\| |1, 1\rangle\| \cdot \|J_- |j, m-1\rangle\|}{\| |1, 0\rangle\| \cdot \| |j, m-1\rangle\|} \\
&= \frac{\lambda}{\sqrt{N}} \|J_- |j, m-1\rangle\| \\
&= \frac{\lambda}{\sqrt{N}} \| [j(j+1) - (m-1)(m-2)]^{\frac{1}{2}} |j, m-2\rangle \| \\
&= \frac{\lambda}{\sqrt{N}} [j(j+1) - (m-1)(m-2)]^{\frac{1}{2}}, \tag{4.11}
\end{aligned}$$

$$\begin{aligned}
\Gamma_{1 \rightarrow 0}(j, m) &= \frac{\lambda}{\sqrt{N}} \frac{\|\sigma_- |1, 1\rangle\| \cdot \|J_+ |j, m-2\rangle\|}{\| |1, 1\rangle\| \cdot \| |j, m-2\rangle\|} \\
&= \frac{\lambda}{\sqrt{N}} \frac{\|[\frac{1}{2}(1(1+1) - 1(1-1))]^{\frac{1}{2}} |1, 0\rangle\| \cdot \|J_+ |j, m-2\rangle\|}{\| |1, 1\rangle\| \cdot \| |j, m-2\rangle\|} \\
&= \frac{\lambda}{\sqrt{N}} \frac{\| |1, 0\rangle\| \cdot \|J_+ |j, m-2\rangle\|}{\| |1, 1\rangle\| \cdot \| |j, m-2\rangle\|} \\
&= \frac{\lambda}{\sqrt{N}} \|J_+ |j, m-2\rangle\| \\
&= \frac{\lambda}{\sqrt{N}} \| [j(j+1) - (m-1)(m-2)]^{\frac{1}{2}} |j, m-1\rangle \| \\
&= \frac{\lambda}{\sqrt{N}} [j(j+1) - (m-1)(m-2)]^{\frac{1}{2}} \tag{4.12}
\end{aligned}$$

and

$$\begin{aligned}
\Gamma_{0 \rightarrow -1}(j, m) &= \frac{\lambda}{\sqrt{N}} \frac{\|\sigma_- |1, 0\rangle\| \cdot \|J_+ |j, m-1\rangle\|}{\| |1, 0\rangle\| \cdot \| |j, m-1\rangle\|} \\
&= \frac{\lambda}{\sqrt{N}} \frac{\|[\frac{1}{2}(1(1+1) + 0(0+1))]^{\frac{1}{2}} |1, -1\rangle\| \cdot \|J_+ |j, m-1\rangle\|}{\| |1, 0\rangle\| \cdot \| |j, m-1\rangle\|} \\
&= \frac{\lambda}{\sqrt{N}} \frac{\| |1, -1\rangle\| \cdot \|J_+ |j, m-1\rangle\|}{\| |1, 0\rangle\| \cdot \| |j, m-1\rangle\|} \\
&= \frac{\lambda}{\sqrt{N}} \|J_+ |j, m-1\rangle\| \\
&= \frac{\lambda}{\sqrt{N}} \| [j(j+1) - (m-1)m]^{\frac{1}{2}} |j, m\rangle \| \\
&= \frac{\lambda}{\sqrt{N}} [j(j+1) - (m-1)m]^{\frac{1}{2}}. \tag{4.13}
\end{aligned}$$

The total jump rate  $\Gamma(j, m)$  is the sum of all allowed jump rates,

$$\Gamma(j, m) = \sum_{\alpha} \Gamma_{\alpha}(j, m).$$

Whether or not a particular jump is allowed is dependant on the state of the central spin. This three level system has a total of four possible jumps. If the central system is in either of the states  $|1, 1\rangle$  or  $|1, -1\rangle$ , only one jump is allowed and care should be taken to note that they are generally unequal. If the central system is in the state

$|1, 0\rangle$ , two jumps are allowed and the total jump rate is their sum, and the jump direction is chosen randomly with the probabilities  $\pi_{0 \rightarrow -1}$  and  $\pi_{0 \rightarrow 1}$ .

After calculating the four jump rates, and using (4.7) along with the definition for the density matrix in the form of an expectation (3.1), the element of the density matrix of the central spins  $\rho_{11}$  can be expressed as

$$\begin{aligned} \rho_{11}(t) &= \langle 1, -1 | \rho_S(t) | 1, -1 \rangle \\ &= E[\langle 1, -1 | \psi_1(t) \rangle \langle \psi_2(t) | 1, -1 \rangle \langle \chi_2(t) | \chi_1(t) \rangle]. \end{aligned} \quad (4.14)$$

It is assumed for the equations above that the initial condition of the system is such that the central spin begins in state  $|\psi(0)\rangle = |1, -1\rangle$ . It is not sufficient in this case that the number of jumps that each of the two states  $|\psi_\nu(t)\rangle$  is even in order for the density matrix element to be considered non-zero, it is also a requirement that the two states  $|\psi_1\rangle$  and  $|\psi_2\rangle$  are both  $|1, -1\rangle$ , since there three rather than just two states possible.

#### 4.2 Algorithm for Spin 1 case

This section details the construction of the algorithm used to simulate the trajectory followed by the density matrix of the central spin's state for the three level system. The first part of the algorithm involves setting up parameters, exactly as in the previous chapter, such as the number of bath spins, the final time until which the simulation will run, and the coupling constant. Additionally, this parameter setup phase is where the probability distribution function for states  $|j, m\rangle$  is set up. The case where the central system is a three level system rather than a simple qubit requires some important changes, however the bath remains unchanged. A cumulative probability distribution function is set up for all possible  $j$  values running from 1 to half the number of bath spins,  $\frac{N}{2}$ . Identically to the previous chapter, the probability of the bath existing in state  $|j, m\rangle$ , given by (2.18), is dependant on  $j$  but not on  $m$ . As a result, the quantum number  $j$  is picked according to this probability but the corresponding quantum number  $m$  is chosen according to a uniform distribution. This is done because each  $m$  is equally likely for any given value of  $j$ .

Once the parameters are set up, the two independently evolving states  $|\psi_1(t)\rangle$  and  $|\psi_2(t)\rangle$  are simulated. One realisation of this simulation involves stepping through time from  $t = 0$  until the final time  $t = t_f$  in steps of the random waiting time

$\tau = \frac{-\log(\eta)}{\Gamma}$  where  $\eta$  is a uniformly distributed number between 0 and 1, and as a result the jumps constitute a Poisson process. Every time a new  $\tau$  is found and added to the existing time, this indicates that a jump occurs. Ensuring that the time does not run past  $t_f$ , a record is kept of when these jumps occur and to which new state the system has jumped. In this case, the system exists in either  $|1, -1\rangle$ ,  $|1, 0\rangle$  or  $|1, 1\rangle$  and so care must be taken since there may be more than one possible state to jump into. As well as recording which state is occupied at each time interval, a record must also be kept of what factors the jumps have contributed to the state's evolution. Recall that every jump contributes a factor  $(-i)$  to  $|\psi\rangle$  and between jumps there is no drift. For  $|\chi\rangle$ , the deterministic drift is the factor  $e^{\Gamma t}$ , but one should note that in this case  $\Gamma(j, m)$  is dependant on the currently occupied state.

Once this procedure has been concluded twice, once for each independently evolving  $|\Phi_\nu(t)\rangle$ , this constitutes one realisation. For each realisation, a new pair of quantum numbers  $j$  and  $m$  are picked for the bath state, and then for this bath state the composite system state is simulated twice, once for each of the two independent  $|\Phi_\nu(t)\rangle$ 's.

If the initial condition is assumed to be  $|\frac{1}{2}, -\frac{1}{2}\rangle$ , the density matrix element  $\rho_{11}(t)$  for a specified time interval can be calculated by averaging over many realisations of the product

$$\langle 1, -1 | \psi_1(t) \rangle \langle \psi_2(t) | 1, -1 \rangle \langle \chi_2(t) | \chi_1(t) \rangle, \quad (4.15)$$

where  $\langle 1, -1 | \psi_1(t) \rangle$  is either 0 or  $(-i)^{n_{j1}}$ , and  $n_{j1}$  is the number of jumps  $|\psi_1(t)\rangle$  has undergone. Similarly,  $\langle \psi_2(t) | 1, -1 \rangle$  is either 0 or  $(+i)^{n_{j2}}$ , where  $n_{j2}$  is the number of jumps  $|\psi_2(t)\rangle$  has undergone. The contributions from  $\langle \chi_2(t) | \chi_1(t) \rangle$  are each just  $e^{\Gamma t}$  but as previously mentioned, one must be careful to remember that  $\Gamma(j, m)$  depends on which state  $\psi(t)$  is in at that time. In the case of the qutrit as the central system, one must use the record of which states were occupied at each time interval to determine the function  $\Gamma$  for each time interval as it will change as the central state changes. Averaging the product of (4.15) with the probability distribution (2.18) over many realisations results in an approximation of the density matrix element which approaches the exact value given enough realisations.

### 4.3 Results

Presented here are the results of running the algorithm described in this study for a three level system. Shown also are the graphs of each analytical expression [23] corresponding to the numerical plots of the density matrix elements in Figure 4.2.

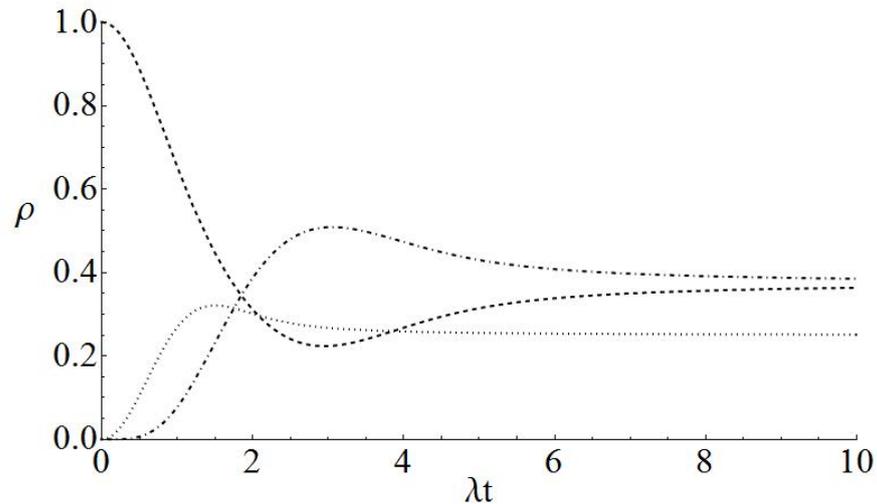


Fig. 4.2: Plot of the analytical expression for the density matrix elements  $\rho_{11}(t)$  (dashed),  $\rho_{22}(t)$  (dotted) and  $\rho_{33}(t)$  (dot-dashed) with the initial condition  $\rho_{11}(0) = 1$ .

It is clear that the numerical plots closely approximate the analytical results, but also evident is the exponential growth of the errors. These analytical results are exactly those for the situation where a pair of spin one-half qubits as the central system interacts with a bath of spin one-half qubits, since the state  $|0, 0\rangle$  remains forever decoupled from the interaction with the bath [23]. As a consequence, this numerical approximation technique is efficient up to  $\lambda t = 1$  and beyond this limit the computational cost of reducing the errors becomes infeasible. In this particular example of the three level system interacting with a spin bath, there is some interesting behaviour that one may notice from the analytical plots. These points of interest, local minima, occur beyond the limit attainable numerically with a reasonable program running time. This is not to say that the results cannot be produced with this program, only that it would require a very large time.

The fact that these local minima are outside the scope of there particular numerical

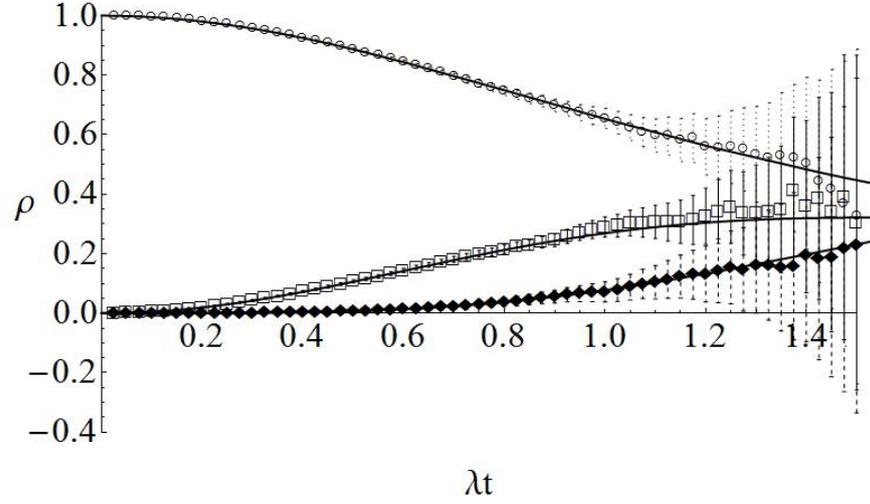


Fig. 4.3: Numerical plot of the density matrix elements  $\rho_{11}(t)$  (circles with dots),  $\rho_{11}(t)$  (squares with lines) and  $\rho_{11}(t)$  (diamonds with dashes) with the initial condition  $\rho_{11}(0) = 1$ , where the simulation was run for  $10^6$  realisations. The analytical solution is represented by the solid line.

plots does not in any way diminish the importance of these results. As previously mentioned, with an investment in significant computational power, this simulation could be run further in  $\lambda t$ . The other important result of these numerical plots is the good agreement with the exact analytical plots which underscores the usefulness of this numerical algorithm which may be applied to situations where an analytical expression may not be possible.

The difference between the case where the central system consists of just one spin half particle, and the case here where the system consists of a spin one particle, or any three level system - a qutrit, is large in terms of the complexity involved in deriving analytical expressions for the dynamics of the central open system. In the case where even more complex systems are studied as the central open system, it becomes much more attractive to use numerical techniques in order to produce plots of the system's time evolution.

A remarkable difference can be seen between Figure 4.3 and 4.4 in that the error bars are significantly smaller when the simulation is run for two orders of magnitude longer. The accuracy of this algorithm is limited only by available computational

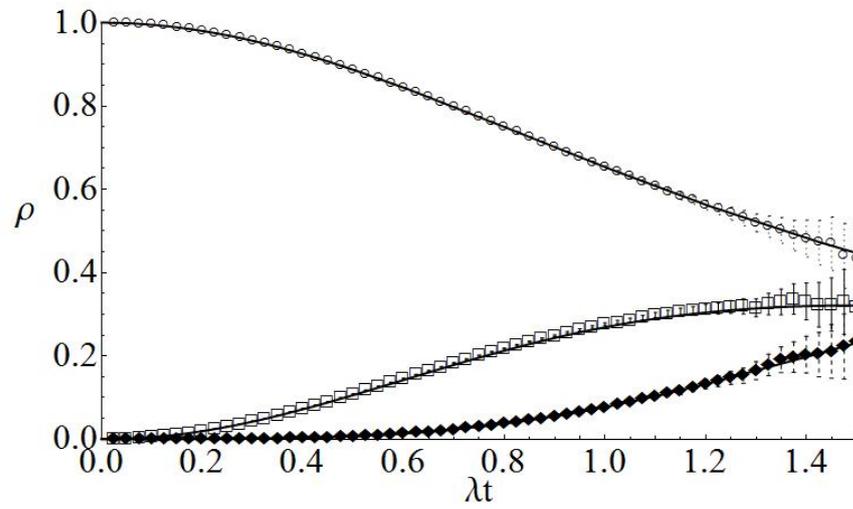


Fig. 4.4: Numerical plot of the density matrix elements  $\rho_{11}(t)$  (circles with dots),  $\rho_{11}(t)$  (squares with lines) and  $\rho_{11}(t)$  (diamonds with dashes) with the initial condition  $\rho_{11}(0) = 1$ , where the simulation was run for  $10^8$  realisations. The analytical solution is represented by the solid line.

time.

To summarise, these results shown here agree very well with the analytical results, and despite the restrictions introduced by the error growth rate on the timespan across which the simulation can be run, it is nevertheless useful in situations where it may not be possible to derive the equations of motion analytically.



## 5. A MEASURE OF NON-CLASSICALITY FOR A STATE

### 5.1 *The Border Between Classical and Quantum*

The theory of quantum mechanics, and also quantum statistical mechanics, has provided many new tools which may be used to describe phenomena which do not obey classical theories. Any new theory should of course agree with currently established theories in the classical limit - the limit as the Planck constant becomes zero. The point at which a line should be drawn between classical and quantum descriptions is very unclear[24]. There have been studies showing, for example, that the Josephson junction should be modeled as a quantum system[25], but there is evidence that it can also be treated as a classical non-linear oscillator[26]. Another example of a system with semiclassical behavior are the so-called Rydberg atoms[27]. Aside from classical behaviour emerging from quantum decoherence, one should remember the Bohr Correspondence Principle which simply argues that *The systems consisting of a large number of particles and/or emerging in quantum states characterised by large quantum numbers behave classically*[28]. Proposed here is a derivation of a witness which can decide whether a given system should be treated as quantum, or whether a classical probabilistic treatment is sufficient. Local hidden variable theories are for this purpose not considered, a system is taken to either be classical or quantum. This is not intended to make a general statement as to the quantum or classical nature of all possible systems, but is of interest, for example, in deciding whether for a given set of experimentally accessible states, with a set of experimentally accessible observables, any quantum behaviour is detectable.

### 5.2 An Example of a Quantum Witness for a Qubit

For some two-dimensional system, for example a qubit, one can express the state using the Bloch representation of its density matrix as

$$\rho = \frac{1}{2}(\mathbb{1} + v_x\sigma_x + v_y\sigma_y + v_z\sigma_z), \quad (5.1)$$

where  $\vec{v}$  is the so-called Bloch vector for the system. In matrix form, this can be written as

$$\rho = \frac{1}{2} \begin{pmatrix} 1 + r \cos(\theta) & e^{i\phi} r \sin(\theta) \\ e^{-i\phi} r \sin(\theta) & 1 - r \cos(\theta) \end{pmatrix}. \quad (5.2)$$

In this representation,  $0 \leq \theta \leq \pi$  is the polar coordinate,  $0 \leq \phi \leq 2\pi$  is the azimuthal coordinate, and  $r$  is the radial coordinate for the Bloch vector. The total space spanned by all Bloch vectors is just the space of all two-dimensional density matrices and in the Bloch representation is a sphere of radius 1.

Equation (5.2) is the most general form of a density matrix for a qubit with  $0 \leq r \leq 1$ . The pure states on the surface of the Bloch sphere are a special case where  $r = 1$ . A state in which  $r = 0$  represents the maximally mixed state  $\rho = \frac{1}{2}\mathbb{1}$ . One may define  $A$  and  $B$  to be operators acting on the density matrix of some system. The operator  $W = B^2 - A^2$  is a witness, where the operators  $A$  and  $B$  are normalised:  $0 < A < B < \mathbb{1}$ . The normalised witness studied here is such that if

$$\text{Tr}\{\rho W\} < 0, \quad (5.3)$$

then the statistics of experimental data obtained by measurements of  $A$  and  $B$  in a state  $\rho$  cannot be described by a classical model. Such a witness, as expected, describes a plane through the Bloch sphere. The conditions  $0 < A < B < \mathbb{1}$  requires that the eigenvalues of  $(B - A)$  be positive, and without loss of generality,  $B$  can be chosen diagonal and such that

$$B = \begin{pmatrix} 1 & 0 \\ 0 & b \end{pmatrix}, \quad (5.4)$$

where  $0 < b < 1$ . The observable  $A$  is then written as

$$A = \begin{pmatrix} a_1 & \xi \\ \xi^* & a_2 \end{pmatrix}. \quad (5.5)$$

Under these conditions, one arrives at the equation

$$\text{Tr}\{W\rho(r, \theta, \phi)\} = \frac{1}{2} (1 - a_1^2 - a_2^2 + b^2 - 2\xi^2) \quad (5.6)$$

$$+ \frac{1}{2} ((1 - a_1^2 + a_2^2 - b^2) r \cos(\theta)) \quad (5.7)$$

$$- (a_1 + a_2) r \xi \cos(\phi) \sin(\theta). \quad (5.8)$$

For any chosen state  $\rho(r, \theta, \phi)$ , one can find a minimum value for this witness, taking this minimum over all experimentally accessible observables  $A$  and  $B$ . In Ref. [29], a minimum value for this witness was found, optimising over all possible observables  $A$  and  $B$  using numerical techniques. These techniques combined random search and simulated annealing algorithms. The choice of parameters for the two observables  $A$  and  $B$  giving this minimum are

$$A = \begin{pmatrix} 0.724 & 0.249 \\ 0.249 & 0.0854 \end{pmatrix}, \quad B = \begin{pmatrix} 1 & 0 \\ 0 & 0.309 \end{pmatrix}, \quad (5.9)$$

and the corresponding eigenstate for the witness  $W$  is

$$\Psi = \begin{pmatrix} 0.391 \\ 0.920 \end{pmatrix}. \quad (5.10)$$

For these parameters, the witness gives the value

$$\langle W \rangle_{\Psi} = -0.0590. \quad (5.11)$$

Using these same parameters for the observables  $A$  and  $B$ , the Bloch sphere of all possible states  $\rho(r, \theta, \phi)$  along with the plane described by  $\text{Tr}\{W\rho(r, \theta, \phi)\}$  is plotted in Figure 5.1. This figure depicts the Bloch sphere; the darker shaded portion, for which  $\text{Tr}\{W\rho\} > 0$ , and the lighter portion, where  $\text{Tr}\{W\rho\} < 0$ , are separated by the plane for which  $\text{Tr}\{W\rho\} = 0$ .

### 5.3 Applications of This Test

The previous section gave an example of how this test can be used for a qubit, but it is also generally applicable in higher dimensions [24]. For the models presented in

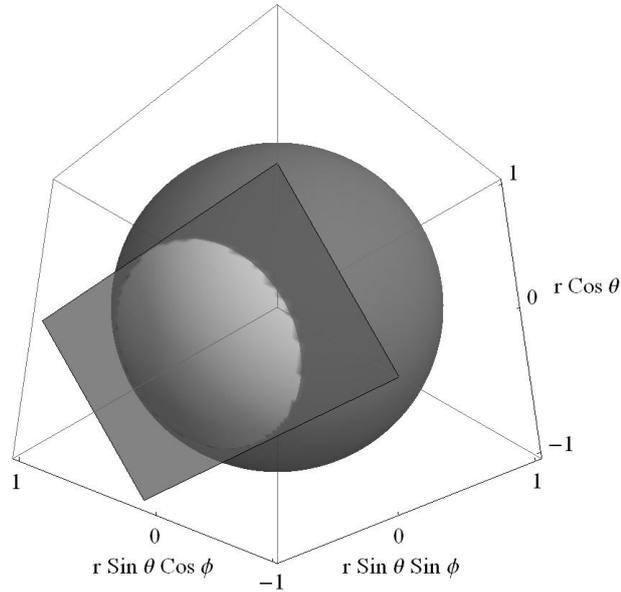


Fig. 5.1: The Bloch sphere representing all possible qubit states with the intersecting plane described by the witness  $W$ . States for which  $\text{Tr}\{W\rho(r, \theta, \phi)\} < 0$  are colored a lighter grey. The parameters used for the witness are those in Equation (5.9)

this study, this test is highly applicable in the sense that one can take density matrices generated by the numerical algorithms shown in previous chapters and explore the behaviour of  $\text{Tr}\{W\rho_{num}(t)\}$ , where  $\rho_{num}(t)$  is some numerically obtained density matrix, with time, for a carefully chosen set of experimentally accessible observables. This method can effectively model whether, for a given system, any quantum effects should be observable. For systems more complex than a qubit model with non-trivial interactions with the environment this method may find use where practical experiments are infeasible.

The method used to implement this involves numerically calculating a minimum for  $\text{Tr}\{W\rho_{num}(t)\}$  across all valid and experimentally accessible observables  $A$  and  $B$ . This is done for many values of  $t$  as multiples of some arbitrarily chosen timestep. The result of this simulation is a measure of detectable quantum behaviour versus time.

## 6. SUMMARY AND CONCLUSION

### 6.1 *Summary*

This Masters thesis began by introducing the reader to the theory and results which would later be used to develop the numerical techniques for exactly solving the dynamics for density matrices. Also in this introduction, many excellent references are given to both introductory and advanced textbooks on the subject of statistical quantum mechanics. The main focus of the introductory chapter is to acquaint the reader with the concepts of closed and open quantum systems, and to present the standard methods used in the study of these systems.

After this introduction, a relevant example was presented in the second chapter - the spin star model. The non-Markovian dynamics of this model was explained, and this model would go on to become the fundamental model used in this study. The spin star model is simple enough that it should not confuse a casual reader, but still retains interesting non-Markovian behaviour.

The third and fourth chapters focused on developing stochastic dynamical equations, and corresponding numerical algorithms, for the density matrix dynamics for a spin half and spin one particle in a spin half environment respectively. In each of these two chapters, the numerical algorithm was explained and derived from the PDP equations of motion for the system. In each of the two cases, the results were compared to the exact analytical solution.

The agreement between the numerical and analytical plots demonstrates the usefulness of the stochastic wavefunction Monte Carlo simulation. Furthermore, for the fourth chapter, a weakness of the technique is pointed out in a limitation of the timescale for which the dynamics of a system can be solved. With both cases, it is demonstrated how accuracy increases with an increase in the number of realisations. The techniques used in this study were shown to be powerful while remaining general enough to be applicable to many different problems.

In Chapter 5, work is presented that has been submitted to a peer reviewed journal

for publication. This work involves a proposed witness of quantumness for a single system. The algorithms in Chapters 3 and 4 are perfectly suited to simulate a system which can be studied with the proposed witness. Although fully implementing such a numerical simulation involves a large amount of computational power, it nevertheless could provide interesting results in further modeling the effects of decoherence and dissipation.

## 6.2 Conclusion

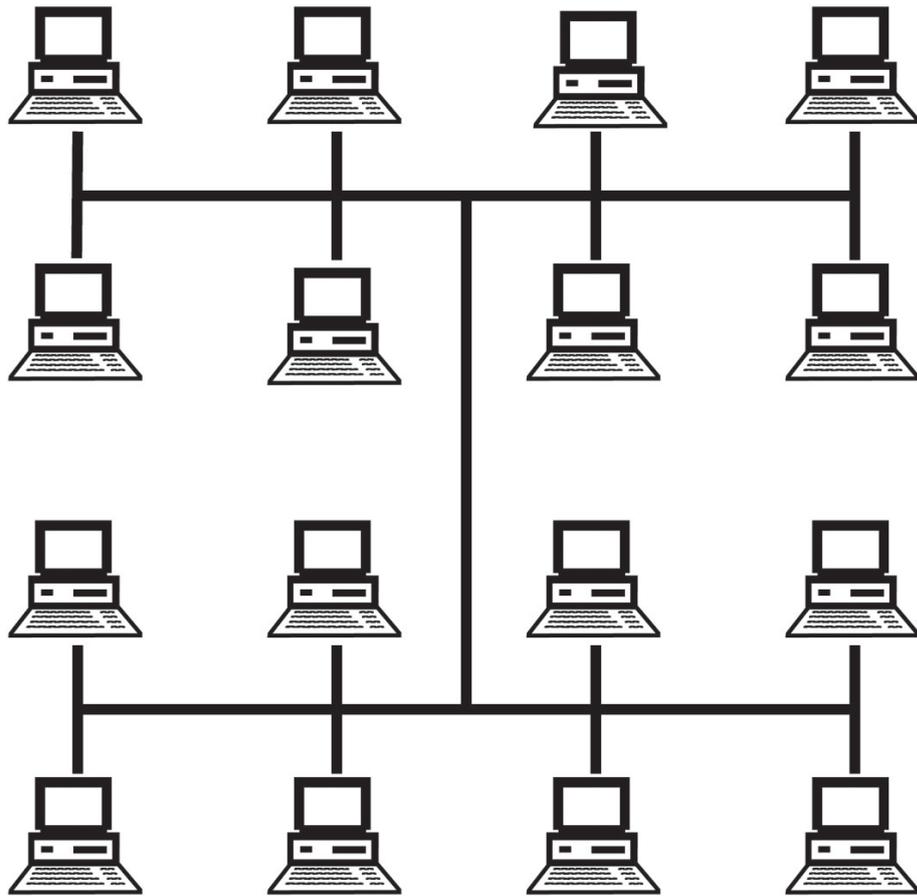
The focus of this study has been on open quantum systems, and specifically on techniques used in numerical simulations of open quantum systems. The spin star model discussed at length in this study is very useful in illustrating various concepts unique to open quantum systems, and is a good example of a problem for which a Markovian description does not suffice. Although this model is relatively simple, it serves to introduce a non-specialist reader to many important tools that one requires to tackle other problems in open quantum systems. The distinction between a closed quantum system and an open system is an important one, and further research in this field will undoubtedly lead to many technical advances in information processing, communication and electronics. The ability to resist decoherence effects in qubits, whether used for data storage, or as a transport channel for communication, is vital to developing and realising practical devices that use quantum algorithms.

As this field of study grows more complex, so does the need for efficient numerical simulations of the systems concerned. This study presents a method of simulating a very general open quantum system and is not restricted to Markovian processes. Numerical techniques as well as analytical analyses of systems enable one to gain a deeper insight into quantum processes and effects and perhaps even develop a stronger intuition, aiding future researchers in developing new ideas.

Ongoing research with the goal of developing quantum computers is attracting great interest from scientists all over the world. The question of how to create quantum gates and registers that can be scaled up to form a useful quantum computer has still not been answered, but examples like the Nitrogen-vacancy color centre in a diamond crystal lattice[30], the double optical lattice[31] and ion traps[32].

A topic not discussed in any detail in this study is the use of parallel computing to run numerical simulations. The Monte Carlo simulation used in this study lends itself very well to massive parallelisation due to the independence of each main loop

iteration. Parallel computing can become important especially since the computing cost of the algorithm in this study increases exponentially with the timespan across which the system's evolution is simulated. If the fastest available hardware is already being used, this is the only means to increase computing power. It can also be a very affordable way of effectively increasing available computing power, as many slower machines may be networked and computing tasks can be split into pieces, each machine in the grid completing their part of the calculations, and finally the results reassembled.



*Fig. 6.1:* A diagram representing a grid of computers networked in such a way as to share computationally heavy tasks, spreading the workload over a grid of nodes resulting in a shorter time to complete the calculations.

The simulations in this study were developed with parallelisation in mind. There are many different implementations of parallel computing but among the scientific

computing community, two popular systems are MPI and OpenMP. For speed and scalability, popular programming languages are C, C++ and FORTRAN. As a result, the simulations in this study have been written in FORTRAN, which is both well known and adheres well enough to current standards that it can be moved across platforms with ease. Additionally, altering the program for use on a parallel computer or grid is very simple.

It is the author's hope that this has provided an introduction into the study of open quantum systems that is both interesting and accessible, and that the reader has gained some insight into the techniques and challenges presented by the problems examined here. The relatively recent development of this field means that it is both challenging and rewarding, and there are still many exciting discoveries still to be made.

## APPENDIX



## A. SIMULATION CODE

What follows below is the FORTRAN code for the numerical simulations in this study. The code was programmed, compiled and run on a Debian Linux system using GNU Fortran 90.

```
1      program SpinStar
2
3      ! %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
4      ! %
5      ! % Stochastic Monte Carlo Simulation
6      ! %
7      ! % Spin Star Environment
8      ! % Surrounding a qubit or qutrit
9      ! %
10     ! %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
11
12     ! Parameters
13     implicit real*8 (a-h,o-q,s-z)
14
15     ! Simulation parameters to be set:
16     parameter(initialstate=1,nstep=40, N=100, nn=N/2)
17
18     double complex phi
19     dimension phi(2,3,nstep+1,2)! The wavefunction phi=psi-cross-chi
20 ! A value is called with phi(instance,state,timestep,component)
21
22     dimension timestep(nstep+1) ! Timesteps dt from t=0 to t=tf
23     double precision iteration
24     double precision epsilon      !Epsilon close to 0
25     double precision realisations !Number of realisations to average
26     double precision srho11
27     double precision srho11error
28     double precision srho12
29     double precision srho12error
30     double precision srho13
31     double precision srho13error
32     double precision srho22
33     double precision srho22error
34     double precision srho23
35     double precision srho23error
36     double precision srho33
37     double precision srho33error
38     dimension F(nn+1)             ! Cumulative PDF for P(j,m)
39     dimension y1(N+1)              !-\
40     dimension y1log(N+1)          !--\ Used to calculate
41     dimension y2(nn+1)            !--/ the PDF and cumulative PDF
42     dimension y2log(nn+1)         !-/
43     dimension prob(nn+1)          !PDF for P(j,m)
44     dimension srho11(nstep+1)
45     dimension srho11error(nstep+1)
46     dimension srho12(nstep+1)
47     dimension srho12error(nstep+1)
48     dimension srho13(nstep+1)
49     dimension srho13error(nstep+1)
```

```

50     dimension srho22(nstep+1)
51     dimension srho22error(nstep+1)
52     dimension srho23(nstep+1)
53     dimension srho23error(nstep+1)
54     dimension srho33(nstep+1)
55     dimension srho33error(nstep+1)
56     integer*4 timeArray(3)    ! Holds the hour, minute, and second
57     integer state
58     integer newstate
59
60     epsilon=2.2204d-16
61
62     ! Another parameter to be set
63     realisations=1.0d6
64
65     A=1.0
66     kdata=9
67     call itime(timeArray)    ! Get the current time
68     seed=rand ( timeArray(1)+timeArray(2)+timeArray(3) )
69
70
71 ! Beginning of program
72
73     ! Last parameter to be set:
74     tf=1.0
75
76     dt=tf/nstep
77     write(*,*) 'Program beginning...'
78 ! Initialise all variables
79     do 14,i=1,nstep+1
80         srho11(i)=(0.0,0.0)
81         srho11error(i)=(0.0,0.0)
82         srho12(i)=(0.0,0.0)
83         srho12error(i)=(0.0,0.0)
84         srho13(i)=(0.0,0.0)
85         srho13error(i)=(0.0,0.0)
86         srho22(i)=(0.0,0.0)
87         srho22error(i)=(0.0,0.0)
88         srho23(i)=(0.0,0.0)
89         srho23error(i)=(0.0,0.0)
90         srho33(i)=(0.0,0.0)
91         srho33error(i)=(0.0,0.0)
92         timestep(i)=dt*i
93 14 continue
94 ! Set up cumulative CDF for picking states |j,m>
95     do 25,i=1,nn+1
96         y2(i)=i
97
98 25 continue
99
100     do 35,i=1,N+1
101         y1(i)=i
102
103 35 continue
104
105
106     do 45,i=1,N
107         y1log(i)=log(y1(i))
108
109 45 continue
110
111
112     do 55,i=1,nn
113         y2log(i)=log(y2(i))
114
115 55 continue
116
117

```

```

118 ! -----
119
120     x = sum(y1log) - 2*sum(y2log) - 2*nn*log(2.0)
121     prob(1) = exp(x)/(nn+1)
122
123     do 65, i=0, nn-1
124         prob(i+2) = prob(i+1)*(2*i+3)**2*(nn-i)/(2*i+1)**2/(nn+i+2)
125 65     continue
126     F(1) = prob(1)
127
128     do 75, i=2, nn+1
129         F(i) = F(i-1) + prob(i);
130 75     continue
131     write(*,*) 'Initialisation complete. Starting main loop..'
132
133 ! -----Start of main loop-----
134     iteration=1
135
136     do 100 while (iteration.LE.realisations)
137         if(mod(iteration,10000.0).EQ.0) then
138             write(*,*) iteration*100/realisations, '% complete'
139         endif
140         do 15, i=1,2
141             do 16 j=1,3
142                 do 17 k=1, nstep+1
143                     do 18 l=1,2
144 ! Reinitialise main array to zeroes
145                     phi(i,j,k,l)=(0.0,0.0)
146
147 18     continue
148 17     continue
149 16     continue
150 15     continue
151
152 ! Select an environment state (j,m) with probability P(j,m)
153     eta=rand(0)
154     j=1
155     do while (j .le. nn .and. eta.GE.F(j))
156         j=j+1
157     end do
158     j=j-1
159     m=floor(rand(0)*(2*j+1))-j
160
161     ! Jump rates for each of the four jumps.
162     ! |1,-1> is 1
163     ! |1,0> is 2
164     ! |1,1> is 3
165     gamma21=sqrt(A*A*real(j*(j+1)-(m)*(m-1))/real(N))+epsilon
166     gamma12=sqrt(A*A*real(j*(j+1)-(m)*(m-1))/real(N))+epsilon
167     !gamma21=sqrt(4.0*A*A*real(j*(j+1)-(m)*(m+1))/real(N))+epsilon
168     !gamma12=sqrt(4.0*A*A*real(j*(j+1)-(m)*(m+1))/real(N))+epsilon
169     gamma23=sqrt(A*A*real(j*(j+1)-(m-2)*(m-1))/real(N))+epsilon
170     gamma32=sqrt(A*A*real(j*(j+1)-(m-2)*(m-1))/real(N))+epsilon
171     !gamma23=0
172     gamma=epsilon !Reinistialise gamma to almost zero
173     state=initialstate ! Starting in state |1,-1>, initial condition
174
175     if(state.EQ.1) then
176
177         if(j.EQ.-m) then ! state |j,m> cannot jump up
178             gamma12=epsilon
179         else if(j.EQ.-m+1) then ! state |j,m> can only jump once
180             gamma23=epsilon
181         endif
182
183     else if(state.EQ.2) then
184         if(-j.EQ.m) then ! state |j,m> cannot jump up
185             gamma23=epsilon

```

```

186     else if(j.EQ.m) then ! state |j,m> can only jump up
187         gamma21=epsilon
188     endif
189
190     else if(state.EQ.3) then
191         if(j.EQ.m) then ! state |j,m> cannot change
192             gamma32=epsilon
193         else if(j.EQ.m-1) then ! state |j,m> can only jump once
194             gamma21=epsilon
195         endif
196
197     endif
198
199 !   Simulating the first Phi. =====
200
201     t=0
202     nj=-1
203     do while (t .LT. tf)
204         nj=nj+1
205         eta = rand(0)
206         if(state.EQ.1) then
207             gamma=gamma12
208             tau = -log(eta)/gamma
209             newstate=2
210         else if(state.EQ.3) then
211             gamma=gamma32
212             tau = -log(eta)/gamma
213             newstate=2
214         else
215             eta2 = rand(0)
216             gamma=gamma21+gamma23
217             tau = -log(eta)/gamma
218             pju=gamma23/gamma
219             newstate=3
220             if(eta2.GE.pju) then
221                 newstate=1
222             end if
223         end if
224 !   We know where what state we are in, and what state we
225 !   are jumping to
226         told=t
227         t=t+tau
228         !write(*,*) "Tau is ",tau," and gamma is ",gamma," eta is ",eta
229 !   We now need to run through timesteps between told and
230 !   tf to update them
231     do 331,i=1,nstep
232         if(timestep(i).GE.told.AND.timestep(i).LE.tf) then
233 !
234             if(i.EQ.1) then
235                 phi(1,1,i,2)=exp(timestep(i)*gamma)
236                 phi(1,2,i,2)=exp(timestep(i)*gamma)
237                 phi(1,3,i,2)=exp(timestep(i)*gamma)
238             else
239
240                 phi(1,1,i,2)=exp(dt*gamma)*phi(1,1,i-1,2)
241                 phi(1,2,i,2)=exp(dt*gamma)*phi(1,2,i-1,2)
242                 phi(1,3,i,2)=exp(dt*gamma)*phi(1,3,i-1,2)
243             end if
244 !
245             =====
246 !
247             =====
248             do 332,i2=1,3
249                 if(i2.EQ.state) then
250                     phi(1,i2,i,1)=(0,-1)**(nj)
251                 else
252                     phi(1,i2,i,1)=(0.0)
253                 end if
254             do 332

```

```

254 ! =====
255
256     end if
257 331   continue
258       state=newstate
259   end do
260
261 ! Repeat this for the other state =====
262 state=initialstate ! Starting in state |1,-1>
263 t=0
264 nj=-1
265 do while (t .LT. tf)
266     nj=nj+1
267     eta = rand(0)
268     if (state.EQ.1) then
269         gamma=gamma12
270         tau = -log(eta)/gamma
271         newstate=2
272     else if (state.EQ.3) then
273         gamma=gamma32
274         tau = -log(eta)/gamma
275         newstate=2
276     else
277         eta2 = rand(0)
278         gamma=gamma21+gamma23
279         tau = -log(eta)/gamma
280         pju=gamma23/gamma
281         newstate=3
282         if (eta2.GE.pju) then
283             newstate=1
284         end if
285     end if
286 ! We know where what state we are in , and what state we are jumping to
287     told=t
288     t=t+tau
289 ! We now need to run through timesteps between told and t update them
290     i=1
291     do while (i.LE.nstep)
292         if (timestep(i).GE.told.AND.timestep(i).LE.t) then
293 ! =====
294             if (i.EQ.1) then
295                 phi(2,1,i,2)=exp(timestep(i)*gamma)
296                 phi(2,2,i,2)=exp(timestep(i)*gamma)
297                 phi(2,3,i,2)=exp(timestep(i)*gamma)
298             else
299                 phi(2,1,i,2)=phi(2,1,i-1,2)*exp(dt*gamma)
300                 phi(2,2,i,2)=phi(2,2,i-1,2)*exp(dt*gamma)
301                 phi(2,3,i,2)=phi(2,3,i-1,2)*exp(dt*gamma)
302             end if
303 ! =====
304 ! =====
305             do 333,i2=1,3
306                 if (i2.EQ.state) then
307                     phi(2,i2,i,1)=(0,1)**(nj)
308                 else
309                     phi(2,i2,i,1)=(0,0)
310                 end if
311             333
312 333   continue
313 ! =====
314     end if
315     i=i+1
316 end do
317 state=newstate
318 end do
319
320 ! Second Phi simulated. End of Realisation. =====
321

```

```

322 ! We now need to simulate the expectation value
323
324 ! Rho11 = <1,-1|rho|1,-1>
325 do 113,i=1,nstep
326
327     srho11(i)=srho11(i)+phi(1,1,i,2)*phi(1,1,i,1)*phi(2,1,i,1)*phi(2,1,i,2)/realisations
328     srho11error(i)=srho11error(i)+((phi(1,1,i,2)*phi(2,1,i,2))**2)/realisations
329
330     srho12(i)=srho11(i)+phi(1,1,i,2)*phi(1,2,i,1)*phi(2,2,i,1)*phi(2,1,i,2)/realisations
331     srho12error(i)=srho11error(i)+((phi(1,1,i,2)*phi(2,2,i,2))**2)/realisations
332
333     srho13(i)=srho11(i)+phi(1,1,i,2)*phi(1,3,i,1)*phi(2,3,i,1)*phi(2,1,i,2)/realisations
334     srho13error(i)=srho11error(i)+((phi(1,1,i,2)*phi(2,2,i,2))**2)/realisations
335
336     srho22(i)=srho22(i)+phi(1,2,i,2)*phi(1,2,i,1)*phi(2,2,i,1)*phi(2,2,i,2)/realisations
337     srho22error(i)=srho22error(i)+((phi(1,2,i,2)*phi(2,2,i,2))**2)/realisations
338
339     srho23(i)=srho11(i)+phi(1,2,i,2)*phi(1,3,i,1)*phi(2,3,i,1)*phi(2,2,i,2)/realisations
340     srho23error(i)=srho11error(i)+((phi(1,1,i,2)*phi(2,2,i,2))**2)/realisations
341
342     srho33(i)=srho33(i)+phi(1,3,i,2)*phi(1,3,i,1)*phi(2,3,i,1)*phi(2,3,i,2)/realisations
343     srho33error(i)=srho33error(i)+((phi(1,3,i,2)*phi(2,3,i,2))**2)/realisations
344
345 113 continue
346
347 ! write(*,*) phi(1,1,10,1)
348 ! write(*,*) phi(2,1,10,1)
349 ! write(*,*) phi(1,1,10,2)
350 ! write(*,*) phi(2,1,10,2)
351
352 ! write(*,*) '_____
353 iteration=iteration+1
354 100 end do
355
356 do 114,i=1,nstep
357
358     srho11error(i)=2*sqrt(srho11error(i)/realisations-srho11(i)**2/realisations)
359     srho12error(i)=2*sqrt(srho12error(i)/realisations-srho12(i)**2/realisations)
360     srho13error(i)=2*sqrt(srho13error(i)/realisations-srho13(i)**2/realisations)
361     srho22error(i)=2*sqrt(srho22error(i)/realisations-srho22(i)**2/realisations)
362     srho23error(i)=2*sqrt(srho23error(i)/realisations-srho23(i)**2/realisations)
363     srho33error(i)=2*sqrt(srho33error(i)/realisations-srho33(i)**2/realisations)
364
365 114 continue
366
367 open (11, FILE='rho11.txt', STATUS='REPLACE')
368 open (12, FILE='rho12.txt', STATUS='REPLACE')
369 open (13, FILE='rho13.txt', STATUS='REPLACE')
370 open (22, FILE='rho22.txt', STATUS='REPLACE')
371 open (23, FILE='rho23.txt', STATUS='REPLACE')
372 open (33, FILE='rho33.txt', STATUS='REPLACE')
373 open (123, FILE='trace.txt', STATUS='REPLACE')
374
375 do 165,i=1,nstep
376
377     write(11,999)timestep(i),srho11(i),srho11error(i)
378     write(12,999)timestep(i),srho12(i),srho12error(i)
379     write(13,999)timestep(i),srho13(i),srho13error(i)
380     write(22,999)timestep(i),srho22(i),srho22error(i)
381     write(23,999)timestep(i),srho23(i),srho23error(i)
382     write(33,999)timestep(i),srho33(i),srho33error(i)
383     write(123,999)timestep(i),srho11(i)+srho22(i)+srho33(i),srho11error(i)+srho22error(i)+srho33error(i)
384
385 999 format(F,F,F)
386
387 165 continue
388     close (kdata)
389

```

```
390     end program SpinStar
```



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