Decoherence by a non-Markovian and non-Gaussian Environment

by

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I hereby declare that I am the sole author of this thesis. This is a true copy of the thesis, including any required final revisions, as accepted by my examiners.

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Abstract

This thesis studies a spin-star model and an open spin-star model. The spin-star model is exactly solvable, and the approximation methods can be applied and compared with the exact solution. As this model is shown to be non-Gaussian and non-Markovian, Born-Markovian approximation is not valid. The comparison of Nakajima-Zwanzig and time-convolutionless methods show that the performances of those two techniques depend on the specific property of the model. The open spin-star model is not exactly solvable and the analytical solution under Gaussian approximation is obtained.

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Chapter 1

Introduction

1.1 Quantum computation

Quantum computing and information theory have became one of the most captivating areas of quantum mechanics in the past two decades [1, 2, 3]. Research into these areas was triggered when Peter Shor [4] showed how a quantum algorithm could super-polynomially accelerate the computations of hard problems more quickly than any known classical algorithm. Besides their mathematical importance, quantum computing and information theory also successfully combine fundamental research into quantum mechanics with modern experimental methods, based on an original idea by Richard Feynman [5]. Those modern experiments include the observation of interference phenomena in Rabi and Ramsey type experiments and also the increase in decoherence times by effective shielding of the experimental setups.

The experimental requirements for the implementation of quantum information processing are daunting as the quantum systems are extremely sensitive to noise from the environment, which causes decoherence of the quantum information. When the error probability of an individual quantum gate is lower than the fault tolerance threshold, which is estimated between 10^{-6} and 10^{-2}, quantum error correction make quantum information processing possible [1, 6].

David DiVincenzo listed a list of requirements [7], called the DiVincenzo criteria, which should be fulfilled by experimental setups to qualify as promising candidates for quantum computing devices:

1. *Scalability*: a physical system with n well characterized qubits,

2. *Initialization*: the ability to prepare the state of the qubits to a pure state, such as $|000\ldots\rangle$,

3. *Stability* : long relevant decoherence times, much longer than the gate operation time,
4. *Ability to control* : a “universal” set of quantum gates,
5. *Ability to measure* : a qubit-specific measurement capability.

1.2 Realization of quantum bits

Several different physical systems have been studied for the experimental realization of quantum bits. The nuclear-magnetic resonance technique (NMR) is the earliest and most developed method [8]. The carriers of quantum information in this physical system are nuclear spins in molecules. Due to the weak coupling between individual spin and the environment, a huge ensemble of spins has to be used and strong magnetic fields have to be applied to the NMR probes. The factorization of 15 into its prime factors 3 and 5 based on a quantum algorithm has been achieved by the NMR technique [9]. Quantum optical implementations of qubits [10, 11] also give good results regarding their impressive decoherence times. They are among the earliest physical systems to realize multipartite entanglement and quantum cryptography. Atomic or molecular energy levels are used to store quantum information and external lasers are used to manipulate the qubit. Based on quantum optical systems, ion traps [12] and optical lattices [13] are also implemented.

The difficulty in scaling up the quantum system from qubits to a many-qubit system has not yet been solved. Although ion trap quantum registers of at most 8 qubits have been achieved, at least 20 to 50 qubits are required to perform non-trivial quantum computations [1, 14]. Solid state qubits based on superconducting technology [15, 16, 17, 18, 19, 20] and quantum dot qubits based on superconducting technology [7, 21] are more promising in order to reach the scalability.

1.3 Qubits and Environments

The main difficulty of implementing the qubit is caused by decoherence [22] , which is given by the interactions between quantum systems and their environments [1]. The combined physical system, the system of interest and its environment, can be considered as a closed system. For example, the time evolution operator of this closed system is unitary. As a result, the decoherence of the central system is due to the entanglement and energy exchange, which give two kinds of decoherence, dephasing and dissipation, respectively. It is important to understand decoherence because quantum computers require long dephasing times for the computations and long dissipation times for the readouts.

1.4 Overview

As mentioned in section 1.3, the unavoidable interaction of quantum system with its environment causes difficulties in the practical realizations of quantum information processing. The quantum coherence could be destroyed and the loss of information could be caused. As a result, it is important to understand the dynamics of open quantum systems in order to avoid the loss of information. The time evolution of closed systems can be represented by the Schrödinger equation; however, the quantum dynamics of an open system cannot be described by unitary time evolution. When the dynamics of an open quantum system are discussed, the equation of motion for its reduced density matrix turns out to be an effective way [23]. There are various exact and approximate approaches that have been developed [24, 23]. However, there are usually practical difficulties to use the exact approaches which often involve complicated integro-differential equations and approximation techniques for the reduced density matrix are practically important.

In this thesis we study two decoherence models: one is an exactly solvable spin-star model, and the other one is an open spin-star model [25, 26]. The spin-star model is the system consisting of a single spin-$\frac{1}{2}$ particle linearly coupled to a bath of spins and the open spin-star model refers to the situation that the spin-star system is coupled to a heat bath. We are motivated by the importance of spin bath models, which usually describe the decoherence in solid state quantum information processors.

In the first part of this thesis, we focus on the study of the spin-star model. The spin-star model is exactly solvable due to its high symmetry, and the reduced dynamics of the central system show that the spin bath is a non-Gaussian and non-Markovian environment. Therefore, this model gives an example for the study of the performances of different non-Markovian techniques. With the help of the exact solution, we are able to discuss the dependences of various parameters, such as the initial state, the number of spins in the spin bath, and the coupling strength, on the time evolution of the reduced system dynamics. In addition, different master equations, which have been developed in the literature, can be studied with the help of the spin-star model. Specifically, in this thesis we discussed the Born and Born-Markov master equations, the Nakajima-Zwanzig (NZ) master equation [27, 28, 29, 30] up to second order in the coupling strength, and the time-convolutionless (TCL) master equation [31, 32] up to fourth order in the coupling strength. As a result, the performance of those approaches can be discussed with the help of comparisons to the exact solution. Although the same spin-star model with similar approaches has been studied in Ref [26], we focus on these studies by introducing collective operators and discussing different observers. In the second part we study the open spin-star model. This model is difficult to be solved analytically in the strong coupling regime. We assume the weak coupling between the central spin and the spin bath, therefore, the spin bath together with heat reservoir can be approximated as a Gaussian environment. The reduced dynamics for the central spin is obtained by using the Gaussian approximation.

This thesis is organized as follows. In chapter 2, we review some definitions critical to the study in this thesis: decoherence, dephasing, quantum irreversibility and recurrence, in the theory of decoherence. Next, we study the pure dephasing model in classical and quantum regime and Gaussian approximations on both regimes. In Chapter 3 we study the spin-star system. The reduced dynamics of the system is exactly solvable and shows non-Gaussian and non-Markovian behavior. The exact solutions for parameters with different values are discussed. We also study various approximation techniques: the Born and the Born-Markov master equations, the Nakajima-Zwanzig (NZ) [27, 28, 29, 30] and the time-convolutionless

[31, 32] projection operator techniques. In Chapter 4 the open spin-star model is studied. The analytical solution with Gaussian approximation for the reduced dynamics of the central spin is derived.

Chapter 2

Definitions and Dephasing Model

2.1 Definitions

2.1.1. Decoherence

The coupling of an open quantum system with its environment causes correlations between the states of the system and the heat bath. These correlations exchange the information between the open quantum system and its environment, which is similar to a quantum probe doing indirect measurement on the open system [23]. The system behaves very differently from its isolated behavior when coupled to the environment. The time-evolution of the open quantum system is not unitary. This environment-induced, dynamic destruction of quantum coherence is called decoherence [22]. In the language of state and density matrix, the superposition of the open quantum system's states is destroyed after tracing over the environmental degrees of freedom and the system's reduced density matrix turns into a statistical mixture. Decoherence is important because long decoherence times are necessary for building quantum computers. As a result, it is crucial to study decoherence mechanisms.

2.1.2 Quantum irreversibility and recurrence

In Ref [33] decoherence is defined restrictively by relating it to the term irreversibility. In addition, irreversibility is related to infinity: a bath of infinite degrees of freedom, i.e., a bath of infinitely many harmonic oscillators could lead to irreversibility [34, 33]. In addition, chaos also causes irreversibility [33]. When the system is coupled with a bath displaying an infinite numbers of freedom, the interacting dynamic is irreversible. The process that transfers energy from the open quantum system to its environment is called *relaxation* or *damping* [35]. The term quantum *dissipation* refers to the process whereby energy flows only from the system to the environment [35]. The dissipation is an irreversible process. Quantum relaxation and dissipation are indistinguishable on a short-time scale, which is much shorter than the relevant time scales. Recurrences, which can lead the quantum state of the interacting systems back to its initial unentangled state, exist in quantum interacting processes. If the time scale of the recurrences is much longer than the duration of any conceivable experiment, the recurrence turns into irreversible decay. Therefore, the time for recurrences of an interaction process depends on the number of degrees of freedom of the bath. When the bath is infinite, the recurrence time is infinite. When the bath is finite, then the recurrence time may be comparable to the relevant time scale and the recurrences need to be considered.

2.2 Dephasing model

In this section we study the basics of dephasing of a qubit introduced by its environment using the pure dephasing models. We are following Chapter 4 of Ref [36].

2.2.1 Classical fluctuating noise

The Hamiltonian of the two-level system reads

$$H = \frac{\Delta}{2}\sigma_z, \tag{2.2.1}$$

where Δ is the energy splitting of the qubit and σ_z is the Pauli matrix of the qubit. The eigenstates $|\uparrow\rangle$ (or $|1\rangle$) and $|\downarrow\rangle$ (or $|0\rangle$) are denoted as excited and ground state. We assume $\hbar = 1$ in this thesis.

The density matrix of the qubit is represented as

$$\rho\left(t\right)=\sum_{i,j=0,1}\rho_{ij}\left(t\right)|i\rangle\langle j|, \tag{2.2.2}$$

where $\rho_{ij}\left(t\right)$ are the density matrix elements in the eigenbasis . The *von Neumann* equation for the qubit,

$$\frac{\partial\rho\left(t\right)}{\partial t}=-i\left[H,\rho\left(t\right)\right], \tag{2.2.3}$$

determines the unitary time evolution of the qubit's density matrix as

$$\rho\left(t\right)=e^{-iHt}\rho\left(0\right)e^{+iHt}. \tag{2.2.4}$$

The qubit is usually coupled to its environment in the practical physical world. When the decoherence is arising from a weak coupling of the qubit to many "fluctuators" in the bath, the central limit theorem (CLT) applies and it is reasonable to assume the fluctuations of the bath yield Gaussian statistics. In addition, "dephasing" is more important than "relaxation" in many low temperature physical systems. We write the Hamiltonian added to the free Hamiltonian of the qubit as

$$H_I=\frac{V\left(t\right)}{2}\sigma_z, \tag{2.2.5}$$

where $V\left(t\right)$ is a stochastic fluctuating variable and $V\left(t\right)=\langle V\rangle+\delta V\left(t\right)$. We assume the fluctuations of V obey Gaussian distribution with zero mean value, $\langle V\rangle=0$.

At this moment, the coupling variable is assumed as a classical variable, and we will show the situation that the qubit is coupled to a quantum fluctuating environment in section 2.2.2.

The longitudinal coupling to the external environment destroys the phase coherence of the qubit, i.e., the diagonal elements of the qubit density matrix is invariant while the off-diagonal elements gain a phase factor such as

$$\rho_{01}(t) = \rho_{01}(0)\, e^{-i\Delta t} e^{i\varphi(t)}, \quad \varphi(t) = -\int_0^t dt^{'} V\left(t^{'}\right). \tag{2.2.6}$$

As a result, this longitudinal coupling model is a *pure dephasing* model. For the Gaussian distributed noise, we have

$$\langle e^{i\varphi}\rangle = e^{i\langle\varphi(t)\rangle - \frac{1}{2}\langle\delta\varphi^2\rangle}, \quad , \delta\varphi(t) = \varphi(t) - \langle\varphi(t)\rangle, \tag{2.2.7}$$

where $\langle\ldots\rangle = \int d\varphi(\ldots)\, p(\varphi, t)$ and it refers to the average over the Gaussian-distributed fluctuations $\delta\varphi$. The probability distribution of $\delta\varphi$, $p(\varphi, t)$, equals $\left(2\pi\langle\delta\varphi^2\rangle\right)^{-1/2} \exp\left(-\delta\varphi^2/\left(2\langle\delta\varphi^2\rangle\right)\right)$. Therefore, the two time correlation function $\langle\delta V(t_1)\, \delta V(t_2)\rangle$ of $\delta V(t)$ determines the phase factor by substituting equation 2.2.7 to 2.2.6:

$$\rho_{01}(t) = \rho_{01}(0)\, e^{-i\Delta t} \exp\left(-\frac{1}{2}\int_0^t dt^{'} \int_0^{t^{'}} dt^{''} \langle\delta V\left(t^{'}\right) \delta V\left(t^{''}\right)\rangle\right). \tag{2.2.8}$$

When the correlations of the environment decay fast enough, in the long time limit the above expression can be approximated as

$$\begin{aligned} \rho_{01}(t) &\approx \rho_{01}(0)\, e^{-i\Delta t} \exp\left(-t\int_{-\infty}^{\infty} dt^{'} \langle\delta V\left(t^{'}\right) \delta V(0)\rangle\right) \\ &= \rho_{01}(0)\, e^{-i\Delta t} e^{-\Gamma_\varphi t}. \end{aligned} \tag{2.2.9}$$

The off-diagonal elements of the system density matrix decay exponentially and the decoherence rate reads

$$\begin{aligned}\Gamma_\varphi &= \int_{-\infty}^{\infty} dt' \langle \delta V\left(t'\right)\delta V\left(0\right)\rangle \\ &= \langle \delta V \delta V\rangle_{\omega=0},\end{aligned} \tag{2.2.10}$$

where the Fourier transform of the correlation function is defined as the noise spectrum:

$$\langle \delta V \delta V\rangle_\omega = \int_{-\infty}^{\infty} dt e^{i\omega t}\langle \delta V\left(t\right)\delta V\left(0\right)\rangle. \tag{2.2.11}$$

2.2.2 Quantum noise

The classical stochastic description of the noise is valid when the environment is at high temperatures. However, the back action of the qubit on its environment should be taking into account and quantum mechanical descriptions are required at low temperatures. We assume the interaction Hamiltonian between the qubit and the quantum heat bath is longitudinal, $\hat{V}\sigma_z/2$, and the total Hamiltonian is

$$H = \frac{\Delta}{2}\sigma_z + \frac{\hat{V}}{2}\sigma_z + H_B. \tag{2.2.12}$$

When the initial state of the whole system is a product state, $\rho_q\left(0\right)\otimes\rho_B\left(0\right)$, one of the off-diagonal elements for the reduced density matrix can be calculated as

$$\begin{aligned}\langle 0|\rho_q\left(t\right)|1\rangle &= \langle 0|Tr_B\left\{e^{-iHt}\rho\left(0\right)e^{iHt}\right\}|1\rangle \\ &= \langle 0|Tr_B\left\{e^{-i\left(\frac{\omega_0}{2}\sigma_z+\frac{\hat{V}}{2}\sigma_z+H_B\right)t}\rho_q\left(0\right)\otimes\rho_B\left(0\right)e^{+i\left(\frac{\omega_0}{2}\sigma_z+\frac{\hat{V}}{2}\sigma_z+H_B\right)t}\right\}|1\rangle \\ &= \langle 0|\rho_q\left(0\right)|1\rangle\cdot e^{-i\omega_0 t}\cdot f\left(t\right),\end{aligned} \tag{2.2.13}$$

where

$$f\left(t\right) = Tr_B\left\{e^{-i\left(\frac{\hat{V}}{2}+H_B\right)t}\rho_B\left(0\right)e^{+i\left(-\frac{\hat{V}}{2}+H_B\right)t}\right\} \tag{2.2.14}$$

Thus, the reduced density matrix for the qubit is

$$\rho\left(t\right) = \left(\begin{array}{cc} \rho_{00}\left(0\right) & \rho_{01}e^{-i\Delta t}f\left(t\right) \\ \rho_{10}e^{i\Delta t}f^{*}\left(t\right) & \rho_{11}\left(0\right) \end{array}\right). \tag{2.2.15}$$

2.3 System-environment models

In order to study the decoherence of the qubits, the quantum systems and their environments need to be modeled theoretically. The open quantum system is usually described by a simple central system, i.e, a two level system or an oscilltor, which is coupled to an environment. There are two kinds of environment: one is described by a set of harmonic oscillators and another one is described by a set of spins. In this thesis, we consider the central system as a two level system.

2.3.1 Harmonic oscillator bath

One of the standard models for studying the dynamics of a two level system in a dissipative environment is the Spin-Boson model [37, 38, 39, 40]: the open quantum system is described by a spin-$\frac{1}{2}$ coupled to a bath of harmonic oscillators .

An example is the qubit collectively coupled to the bath modes such that

$$\hat{H}_I = \sum_j \hat{S}_j \otimes \hat{B}_j = \hat{\sigma}_z \otimes \hat{X}\left(t\right), \tag{2.3.1}$$

where $\hat{S}_j$ are the system operators, $\hat{B}_j$ are the bath operators and $\hat{X}(t)$ is a collective bath operator. The collective bath operator, $\hat{X}$, can be expressed in terms of bath modes' coordinate, $\hat{q}_i$ [40]

$$\hat{X}(t) = \sum_i c_i \hat{q}_i. \tag{2.3.2}$$

Therefore, the Spin-Boson Hamiltonian in the second quantization has the form

$$H = \frac{1}{2}\left(\epsilon\hat{\sigma}_x + \Delta\hat{\sigma}_z\right) + \frac{1}{2}\hat{\sigma}_z \otimes \sum_i^N \hbar\lambda_i \left(a_i + a_i^\dagger\right) + \sum_i^N \hbar\omega_i a_i^\dagger a_i, \tag{2.3.3}$$

where $a_i^\dagger$ and a_i are the bosonic creation and annihilation operators of i-th bath mode, $\hat{\sigma}_x$ and $\hat{\sigma}_z$ are the Pauli matrices of the central spin. One can denote the eigenstates of $\hat{\sigma}_z$ by $|0\rangle$ and $|1\rangle$. The energy eigenvalues of the spin-$\frac{1}{2}$ are $\pm E/2$ with $E = \sqrt{\epsilon^2 + \Delta^2}$.

The microscopic parameters of each harmonic oscillator are connected to the macroscopic parameters by introducing the spectral density function $J(\omega)$, and the properties of the bath can be fully characterized by $J(\omega)$. For example[40],

$$J(\omega) = \sum_i \lambda_i^2 \delta(\omega - \omega_i) = \frac{\pi}{2}\sum_{i=1}^N \frac{c_i^2}{m_i\omega_i}\delta(\omega - \omega_i), \tag{2.3.4}$$

where ω_i is the resonance frequency of the i-th oscillator.

2.3.2 Spin bath

The harmonic oscillator environment is very important for modeling the decoherence dynamics with Gaussian environments [39]; however, some other non-Gaussian noise sources can not be modeled by a harmonic oscillator bath.

When the physical systems are at very low temperature, experiments show that the decoherence is typically dominated by coupling with localized modes, e.g, the hopping background charges or general quantum bistable fluctuators in superconducting qubits [41, 42, 43, 44, 45], nuclear spins[46], tunneling charges, defects and paramagnetic electronic impurities. Therefore, these localized modes could be described as finite-dimensional Hilbert spaces with finite energy cutoffs and could be mapped onto an environment of spin-$\frac{1}{2}$ particles [47]. The spin bath model can be applied to various physical systems, such as magnetic systems where the interactions are strong and superconducting systems[47].

Chapter 3

The Spin-Star Model

In th is chapter we study a simple spin star model, which consists a single central spin-$\frac{1}{2}$ system interacting with an environment of N spin-$\frac{1}{2}$ particles [26, 25]. The central spin is located at the center of the whole system and equally coupled to N bath spins. The bath spins are not coupled with each other. The central spin and its environment live in a two-dimensional Hilbert space $\mathcal{H}_{\mathcal{S}}$ and an N-fold tensor product of two dimensional spaces $\mathcal{H}_{\mathcal{B}}$, respectively. In this thesis, we consider an Ising spin-star model which has a diagonal interaction Hamiltonian. This model is exactly solvable due to its high symmetry, so limit situations and approximation methods can be applied and compared with the exact solution. This model is particularly useful to study the spin bath [47] used to describe the decoherence of solid state qubits, i.e., quantum dots spin qubits [7, 17, 48] and the nitrogen-vacancy center in diamond [49, 50].

Some similar spin-star systems have already been studied in Ref [26, 51, 52, 53] , where the analytical solutions are obtained and approximation techniques are applied. For example, in Ref [51] a spin-star model with XY exchange-type and in Ref [26] an Ising model with arbitrary coupling constants are studied. Although in Ref [26] the Ising spin-star model with equal coupling strength has been discussed and various approximation methods are studied, we focus on the methods based on collective operators [25, 54, 55, 56].

When the correlation time of the environment is much shorter than the characteristic time of the system, the correlation function can be assumed to be a δ function under Markovian approximation, which suggests that we can neglect the memory effect from the environment during the evolution of the central system [23]. However, the correlation function of the bath is constant and the correlation time is infinite for our spin-star model, which implies the reduced dynamics of the central spin is non-Markovian.

This chapter is organized as follows. Section 3.1 demonstrates the model and introduces the collective operators. Section 3.2 discusses the exact solutions for three different factorized initial states: spin bath at thermal equilibrium state, spin bath at unpolarized state, and spin bath at ground state. In section 3.3 the short-time limit is studied for the decoherence factor when the initial state of the spin bath is a thermal equilibrium state at temperature T. In section 3.4, firstly, the Born approximation is applied and Markovian approximation is demonstrated to be not applicable; secondly, Nakajima-Zwanzig (NZ) up to second order and Time-convolutionless (TCL) up to fourth order projection operator techniques are applied to the factorized initial state with spin in thermal equilibrium state at finite temperature T. The exact and approximation solutions with various parameters are plotted in section 3.5. Finally, the discussions and conclusions are presented in section 3.6.

3.1 The model

The interaction Hamiltonian of the Ising spin-star model is

$$\hat{H}_I = \hat{\sigma}_z \otimes \sum_{i}^{N} \frac{\lambda_i}{2} \hat{\sigma}_z^{(i)}, \tag{3.1.1}$$

where $\hat{\sigma}_z$ is the Pauli operator for systems, $\hat{\sigma}_z^{(i)}$ is the Pauli operator for i-th bath spin, λ_i is the coupling strength between the central spin and i-th bath spin.

The free Hamiltonians for the central spin and the spin bath are

$$\hat{H}_S = \frac{1}{2}\omega_0 \hat{\sigma}_z \tag{3.1.2}$$

and

$$\hat{H}_B = \sum_{i=1}^{N} \frac{1}{2}\Omega_i \hat{\sigma}_z^{(i)}, \tag{3.1.3}$$

where ω_0 and Ω_i are the energy splitting of the central spin and the i-th spin in the spin bath, respectively. In this thesis, we use $\hbar = k_B = 1$ and we are particularly interested in the situation where the bath spins have identical energy splitting and are equally coupled to the central spin. The collective bath angular momentum operator can be introduced because the individual spin properties can be deducted from the large pseudo-spin operators.

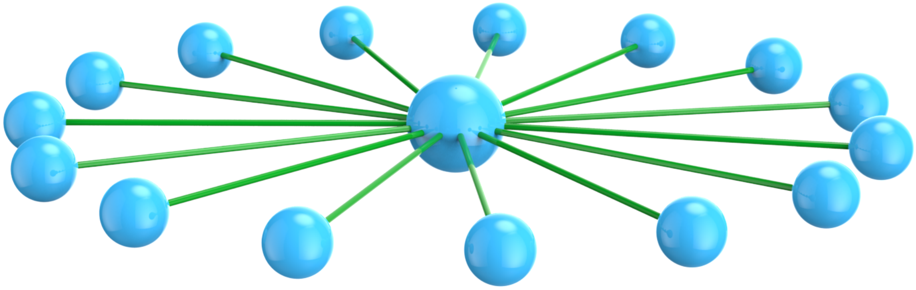

Figure 3.1.1: The diagram of spin-star configuration consisting a single central spin-$\frac{1}{2}$ system equally coupled with N spin-$\frac{1}{2}$ in the spin bath. The spins in the bath are not coupled to one another.

The N spin-$\frac{1}{2}$ can be added to a single large pseudo-spin with angular momentum operators through [25, 54, 55, 56].

$$\hat{J}_x = \frac{1}{2}\sum_{i=1}^{N}\hat{\sigma}_x^{(i)},\;\; \hat{J}_y = \frac{1}{2}\sum_{i=1}^{N}\hat{\sigma}_y^{(i)},\;\; \hat{J}_z = \frac{1}{2}\sum_{i=1}^{N}\hat{\sigma}_z^{(i)}. \tag{3.1.4}$$

Because

$$\hat{\sigma}_{\pm}^{(i)} \equiv \left(\hat{\sigma}_x^{(i)} \pm \hat{\sigma}_y^{(i)}\right) \tag{3.1.5}$$

describes the raising and lowering operators of the i-th bath spin,

for collective large spin operators we have

$$\hat{J}_{\pm} = \hat{J}_x \pm i\hat{J}_y, \ \left[\hat{J}_z, \hat{J}_{\pm}\right] = \pm\hat{J}_{\pm}, \ \left[\hat{J}_+, \hat{J}_-\right] = 2\hat{J}_z. \tag{3.1.6}$$

The eigenstates of $\hat{J}_z$ and $\hat{J}^2$ are defined as Dicke states [57] $|\lambda, j, m\rangle$:

$$\begin{aligned} \hat{J}_z|\lambda, j, m\rangle &= m|\lambda, j, m\rangle && (3.1.7)\\ \hat{J}^2|\lambda, j, m\rangle &= j\left(j+1\right)|\lambda, j, m\rangle, && (3.1.8) \end{aligned}$$

and we have

$$\hat{J}_+|\lambda, j, m\rangle = \begin{cases} \sqrt{\left(j-m\right)\left(j+m+1\right)}|\lambda, j, m+1\rangle & -j \leq m < j \\ 0 & m = j, \end{cases} \tag{3.1.9}$$

$$\hat{J}_-|\lambda, j, m\rangle = \begin{cases} \sqrt{\left(j+m\right)\left(j-m+1\right)}|\lambda, j, m-1\rangle & -j \leq m < j \\ 0 & m = j, \end{cases} \tag{3.1.10}$$

where $\hat{J}^2 = \hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2$ is the total angular momentum squared and j the cooperation number. The allowed values of j are $\left(0, \frac{1}{2}\right), \left(1, \frac{3}{2}\right), \ldots, N/2$ and the allowed values of m are $-j, -j+1, \ldots j$.

The total number of permitted (j, m) values is $\left(N/2+1\right)^2$ for N even and $\left[\left(N+1\right)/2+1\right]\left(N+1\right)/2$ for N odd. The parameter λ is introduced to distinguish the degenerate state $|j, m\rangle$ in eigenspace $\mathcal{M}_{j,m}$. The dimension of $\mathcal{M}_{j,m}$ is $n\left(j, N\right)$ which reads [58, 59, 60]

$$\begin{aligned} n\left(j,N\right) &= \left(\begin{array}{c} N \\ N/2-j \end{array}\right) - \left(\begin{array}{c} N \\ N/2-j-1 \end{array}\right) \\ &= \frac{N!}{\left(\frac{N}{2}-j\right)!}\frac{2j+1}{\left(\frac{N}{2}+j+1\right)!}. \end{aligned} \tag{3.1.11}$$

Therefore, the total Hamiltonian can be written as

$$\hat{H} = \frac{\omega_0}{2}\hat{\sigma}_z + \lambda\hat{\sigma}_z \otimes \hat{J}_z + \Omega\hat{J}_z, \tag{3.1.12}$$

where the central spin couples to the collective angular momentum J_z of N spin-$\frac{1}{2}$.

We assume that for $t < 0$ the system and the environment are decoupled:

$$\rho\left(0\right) = \rho_q\left(0\right) \otimes \rho_B\left(0\right), \tag{3.1.13}$$

where $\rho_{q,B}\left(0\right)$ are density matrices in $\mathcal{H}_{q,B}$, and the state $\rho_q\left(0\right)$ of the system is pure: $|\psi\rangle = \cos\frac{\theta}{2}|0\rangle + \sin\frac{\theta}{2}e^{i\phi}|1\rangle$.

3.2 Exact solution for the spin star model

The reduced density matrix describes the state of the central spin is

$$\rho_q\left(t\right) = \mathrm{Tr}_B\left\{\rho\left(t\right)\right\}, \tag{3.2.1}$$

where Tr_B is the partial trace over the degrees of the freedom of the bath and $\rho\left(t\right)$ is the density matrix for the total system at time t. The density matrix $\rho\left(t\right)$ evolutes under the unitary evolution:

$$\rho\left(t\right)=e^{-iHt}\rho\left(0\right)e^{+iHt}.$$

One of the off-diagonal system density matrix elements in the eigenbasis of the central spin Hamiltonian is

$$\begin{aligned}\langle 0|\rho_q\left(t\right)|1\rangle &= \langle 0|Tr_B\left\{e^{-iHt}\rho\left(0\right)e^{iHt}\right\}|1\rangle \\ &= \langle 0|Tr_B\left\{e^{-i\left(\frac{\omega_0}{2}\hat{\sigma}_z+\lambda\hat{\sigma}_z\otimes\hat{J}_z+\Omega\hat{J}_z\right)t}\rho_q\left(0\right)\otimes\rho_B\left(0\right)e^{+i\left(\frac{\omega_0}{2}\hat{\sigma}_z+\lambda\hat{\sigma}_z\otimes\hat{J}_z+\Omega\hat{J}_z\right)t}\right\}|1\rangle \\ &= \langle 0|\rho_q\left(0\right)|1\rangle\cdot e^{-i\omega_0 t}\cdot Tr_B\left\{e^{-i(\lambda+\Omega)\hat{J}_z t}\rho_B\left(0\right)e^{+i(-\lambda+\Omega)\hat{J}_z t}\right\} \\ &= \langle 0|\rho_q\left(0\right)|1\rangle\cdot e^{-i\omega_0 t}\cdot f\left(t\right) \qquad (3.2.2)\end{aligned}$$

where $f\left(t\right)$ is the decoherence factor defined in chapter 2.

The decoherence factor for another off-diagonal matrix element is

$$\langle 1|\rho_q\left(t\right)|0\rangle=\langle 1|\rho_q\left(0\right)|0\rangle\cdot e^{+i\omega_0 t}f^*\left(t\right). \qquad (3.2.3)$$

Note that the diagonal matrix elements are stationary in this pure dephasing model:

$$\langle 0|\rho_q\left(t\right)|0\rangle=\langle 0|\rho_q\left(0\right)|0\rangle, \qquad (3.2.4)$$

and

$$\langle 1|\rho_q\left(t\right)|1\rangle=\langle 1|\rho_q\left(0\right)|1\rangle. \qquad (3.2.5)$$

a. The initial state of spin bath is in the thermal equilibrium at a finite temperature T

When the spin bath is in the thermal equilibrium state at temperature T, the density matrix of the spin bath is described by

$$\rho_B\left(0\right)=e^{-\beta H_B}/Z, \qquad (3.2.6)$$

where $\beta = 1/k_B T$, Z is the partition function $\mathrm{Tr}_B\left(e^{-\beta H_B}\right)$, and k_B is the Boltzmann constant. We assume k_B is 1 in this thesis.

In the eigenbasis of J_z and J^2 $\{|\lambda, j, m\rangle\}$, the initial density matrix of spin bath, $\rho_B(0)$, reads

$$\begin{aligned}\rho_B(0) &= \frac{1}{Z} e^{-\beta\Omega J_z} \\ &= \frac{1}{Z}\sum_j n(j,N)\left(\sum_{m=-j}^{m=j} e^{-\beta\Omega m}|\lambda, j, m\rangle\langle\lambda, j, m|\right), \qquad (3.2.7)\end{aligned}$$

and the partition function reads

$$Z = \mathrm{Tr}_B\left\{\sum_j n(j,N)\left(\sum_{m=-j}^{m=j} e^{-\beta\Omega m}|\lambda, j, m\rangle\langle\lambda, j, m|\right)\right\}. \qquad (3.2.8)$$

Note that the bath state is stationary under this interaction: $\rho_B(t) = \rho_B(0)$, which is because $\rho_B(t)$ commutes with the interaction Hamiltonian H_I. The exact solution for decoherence factor is obtained from equation 3.2.2 by calculating the traces over spin bath in the eigenbasis of J_z and J^2, $\{|\lambda, j, m\rangle\}$:

$$\begin{aligned}f(t) &= \frac{1}{Z}\sum_j n(j,N)\left(\sum_{m=-j}^{j} e^{-(2i\lambda t+\beta\Omega)m}\right) \qquad (3.2.9)\\ &= \frac{1}{Z}\sum_j n(j,N)\frac{\sin\left[\left(j+\frac{1}{2}\right)(2\lambda t - i\beta\Omega)\right]}{\sin\left(\frac{1}{2}(2\lambda t - i\beta\Omega)\right)}, \qquad (3.2.10)\end{aligned}$$

where λ is the coupling strength, β equals $1/k_B T$, and Ω is the energy splitting of spins in the spin bath.

Equation 3.2.9 is the exact expression of the decoherence factor. It is a sum of finite number of functions

$$\frac{\sin\left[\left(j+\frac{1}{2}\right)\left(2\lambda t-i\beta\Omega\right)\right]}{\sin\left(\frac{1}{2}\left(2\lambda t-i\beta\Omega\right)\right)},$$

which is a periodic function. The frequency of the numerator λ is slow compared to the frequency of the fraction $(2j+1)\,\lambda$ and is perceived as a pitch. In short, it is perceived as a periodic variation of the fraction function (the numerator function is an envelope for the fraction function). As a result, the decoherence factor is also a periodic function and the periods are determined by the coupling strength λ, the number of spins in the spin bath N, and the constant $\beta\Omega$. The coupling strength λ determines the slow frequency and the period of a full recurrence, N and $\beta\Omega$ together determine the fast oscillations in a full recurrence period. Because $\beta\Omega$ is determined by the initial state of environment, the decoherence factor is affected by the initial state of the spin bath. As a periodic function will always return to its initial value, 1, at some time, this decoherence process is fully reversible due to the finite environment. In addition, the decoherence factor does not have an equilibrium value and the central spin does not have an equilibrium state. In summary, the interaction process between the central spin and the spin bath is non-Markovian and has a quantum memory effect.

In this model the bath correlation functions can also be calculated exactly. Because the heat bath density matrix is stationary, the k^{th} order bath correlation function is easily calculated

$$\begin{aligned} Q_k &= Tr_B\left\{J_z^k\rho_B\right\} \\ &= \frac{1}{Z}\sum_j n\left(j,m\right)\left(\sum_{m=-j}^{j} m^k e^{-\beta m\Omega}\right). \end{aligned} \tag{3.2.11}$$

Usually, Q_1 refers to the expectation value of bath operator J_z. The bath correlation functions are time independent due to the stationary bath density matrix and the corresponding bath correlation time is infinitely long.

b. The initial state of the spin bath is an unpolarized state ($T = \infty$).

When the initial state of the spin bath is the thermal equilibrium state at infinitely high temperature, i.e., $T = \infty$ ($\beta \sim 0$), the initial state of the total system is given by an uncorrelated product state $\rho_S(0) \otimes \rho_B(0)$ with

$$\rho_B(0) = 2^{-N} I_B. \tag{3.2.12}$$

Here, I_B refers to the unit matrix in $\mathcal{H}_B$.

The bath state is also stationary under this interaction: $\rho_B(t) = \rho_B(0)$, because $\rho_B(0)$ commutes with the interaction Hamiltonian H_I. The exact solution for decoherence factor is obtained from equation 3.2.2 by calculating the trace over spin bath in the eigenbasis of J_z and J^2:

$$\begin{aligned} f(t) &= \frac{1}{Z} Tr_B \left\{ e^{-2i\lambda \hat{J}_z t} \rho_B(0) \right\} \\ &= \frac{1}{2^{-N}} \sum_j n(j, N) \cdot \left(\sum_{m=-j}^{m=j} e^{-2i\lambda m t} \right) \\ &= \frac{1}{2^{-N}} \sum_j n(j, N) \frac{\sin[(2j+1)\lambda t]}{\sin(\lambda t)}. \end{aligned} \tag{3.2.13}$$

Equation 3.2.13 is the exact expression of the decoherence factor for the situation that the initial state of the bath is an unpolarized state. Similar to the finite temperature case discussed in part a, it is also a sum of finite number of periodic functions

$$\frac{\sin[(2j+1)\lambda t]}{\sin(\lambda t)}.$$

Similarly, we can conclude that the coupling strength λ determines the period of a full recurrence. For this situation, the bath correlation functions can also be calculated exactly.

Because the heat bath density matrix is stationary, the k^{th} order bath correlation function is easily calculated as

$$\begin{aligned} Q_k &= Tr_B\left\{J_z^k \rho_B\right\} \\ &= \frac{1}{2^{-N}} \sum_j n\left(j, m\right)\left(\sum_{m=-j}^{j} m^k\right). \end{aligned} \tag{3.2.14}$$

It is easy to read the information from equation 3.2.14: the bath correlation functions are time-independent and the corresponding bath correlation time is infinitely long.

c. The initial state of the spin bath is its ground state $(T = 0)$

When the initial state of the spin bath is the thermal equilibrium state at absolute zero temperature, i.e., $T = 0$ $(\beta = \infty)$, there is no excitation exist and all the spins in the spin bath are in their down state.

The initial state of the total system is given by an uncorrelated product state $\rho_S\left(0\right) \otimes \rho_B\left(0\right)$ and

$$\rho_B\left(0\right) = |\lambda, \frac{N}{2}, -\frac{N}{2}\rangle\langle\lambda, \frac{N}{2}, -\frac{N}{2}|. \tag{3.2.15}$$

The exact solution for decoherence factor is obtained from equation 3.2.2 by calculating the traces over spin bath in the eigenbasis of J_z and J^2:

$$\begin{aligned} f\left(t\right) &= Tr_B\left\{e^{-2i\lambda\hat{J}_z t}\rho_B\left(0\right)\right\} \\ &= e^{-i\lambda N t} \end{aligned} \tag{3.2.16}$$

The k^{th} order bath correlation function is easily calculated

$$\begin{aligned} Q_k &= Tr_B\left\{J_z^k \rho_B\right\} \\ &= \left(-\frac{N}{2}\right)^k . \end{aligned} \tag{3.2.17}$$

It is easy to read the information from equation 3.2.17: the bath correlation functions are time-independent and the corresponding bath correlation time is infinitely long.

For all of the initial conditions introduced in this section, the slow frequency of the decoherence factors, which gives full recurrences periodically, is independent of the number of spins in the bath, N, and determined by the coupling strength λ. In short, the envelope recurrence period is determined by the coupling strength λ. Note that this is different from the infinite degrees of freedom situation because we could write the bath Hamiltonian as a single collective operator and the degrees of freedom of the bath is reduced.

3.3 Short time behavior

In this section we will study the short-time behavior for the spin star model with the initial state of spin bath is in thermal equilibrium at a finite temperature T.

When the interaction between the central spin and the spin bath is on only for a short time compared to the scale of recurrence period, $\lambda t \ll 1$, the decoherence factor can be expanded and approximated as

$$\begin{aligned} f\left(t\right) &= \frac{1}{Z}\sum_j n\left(j,N\right)\sum_{m=-j}^{j} e^{-2i\lambda m t} e^{-\beta m \Omega} \\ &= \frac{1}{Z}\sum_j n\left(j,N\right)\sum_{m=-j}^{j}\left(1+\left(-2i\lambda m t\right)+\frac{\left(-2i\lambda m t\right)^2}{2!}+\frac{\left(-2i\lambda m t\right)^3}{3!}+\cdots\right) e^{-\beta m \Omega} \\ &= 1-2i\lambda t Q_1 - 2\lambda^2 t^2 Q_2 + \frac{4}{3} i\lambda^3 t^3 Q_3 + \cdots \\ &\approx e^{-2i\lambda t Q_1 - 2\lambda^2 t^2 Q_2}, \end{aligned} \tag{3.2.18}$$

where Q_1 and Q_2 are defined in equation 3.2.11.

Then the off-diagonal elements of the central spin density matrix at a short time become

$$\rho_{S,01}(t) \approx \rho_{S,01}(0)\, e^{-i\omega_0 t} e^{-2i\lambda t Q_1 - 2\lambda^2 t^2 Q_2},$$
$$\rho_{S,10}(t) \approx \rho_{S,01}(0)\, e^{+i\omega_0 t} e^{+2i\lambda t Q_1 - 2\lambda^2 t^2 Q_2}. \tag{3.2.19}$$

3.3 Open Quantum System Approaches

In this section, various open quantum system methods are studied and applied to the spin-star system. The theory part of this section follows Ref [23], which is an excellent reference for studying open quantum system. The master equations for the reduced system density matrix are derived for the initial state of the spin bath is in thermal equilibrium state at temperature T.

We start with considering the central spin system S weakly coupled to the spin bath B. The Hamiltonian of the whole system is assumed to be of the form

$$H(t) = H_S \otimes I_B + I_S \otimes H_B + H_I(t), \tag{3.3.1}$$

where H_S is the free Hamiltonian of the open system S, H_B is the self-Hamiltonian of the environment B, and $H(t)$ is the interaction Hamiltonian between the system and the environment.

In the interaction picture, the von Neumann equation for the total density matrix $\rho(t)$ is:

$$\frac{d}{dt}\rho(t) = -i\left[H_I(t), \rho(t)\right]. \tag{3.3.2}$$

Note we have omit the index I which used to indicate the interaction picture. Equivalently, the interaction picture von Neumann equation can be written in its integral form

$$\rho(t) = \rho(0) - i \int_0^t ds \left[H_I(s), \rho(s)\right]. \tag{3.3.3}$$

Inserting the integral form 3.3.3 into equation 3.3.2 and taking the trace over the spin bath we have

$$\frac{d}{dt}\rho_S(t) = -iTr_B\left[H_I(t), \rho(0)\right] - \int_0^t dsTr_B\left[H_I(t), \left[H_I(s), \rho(s)\right]\right]. \tag{3.3.4}$$

Note that we do not assume $Tr_B\left[H_I(t), \rho(0)\right] = 0$ in this thesis.

a. Born approximation

In order to eliminate $\rho(t)$ from the equation of motion, the Born approximation is performed. This approximation assumes that the coupling between the central system and the bath is weak, so that the influence of the central system on the bath is small. Because the density matrix of the bath ρ_B is only insignificantly affected by the interaction, the density matrix of the whole system at time t can be approximately written as a product state

$$\rho(t) \approx \rho_S(t) \otimes \rho_B. \tag{3.3.5}$$

A closed integro-differential equation for the reduced density matrix $\rho_S(t)$ can be obtained by inserting the product state into the exact equation of motion:

$$\dot{\rho}_S(t) = -iTr_B\left[H_I(t), \rho_S(0) \otimes \rho_B\right] - \int_0^t dsTr_B\left\{\left[H_I(t), \left[H_I(s), \rho_S(s) \otimes \rho_B\right]\right]\right\}. \tag{3.3.6}$$

The integral equation 3.3.6 can be solved easily as the interaction Hamiltonian in our model does not depend on time. We get

$$\dot{\rho}_S\left(t\right) = -i\lambda Q_1\left[\sigma_z, \rho_S\left(0\right)\right] - 2\lambda^2 Q_2 \int_0^t ds\left(\rho_S\left(s\right) - \sigma_z \rho_S\left(s\right)\sigma_z\right), \tag{3.3.7}$$

where Q_1 and Q_2 are the expectation value of bath operator J_z and the second order bath correlation function, respectively, defined in equation 3.2.11.

The equation for decoherence factor $f\left(t\right)$ obtained by using Born approximation reads

$$\dot{f}\left(t\right) = -2i\lambda Q_1 t f\left(0\right) - 4\lambda^2 Q_2 \int_0^t ds f\left(s\right). \tag{3.3.8}$$

Taking the Laplace transform of this integro-differential equation, it becomes

$$sF\left(s\right) - f\left(0\right) = -2i\lambda Q_1 \frac{f\left(0\right)}{s} - 4\lambda^2 Q_2 \frac{F\left(s\right)}{s}, \tag{3.3.9}$$

where $F\left(s\right)$ is the Laplace transform of $f\left(t\right)$. By rearranging the terms, the above equation becomes

$$F\left(s\right) = f\left(0\right)\frac{s - 2i\lambda Q_1}{s^2 + 4\lambda^2 Q_2}. \tag{3.3.10}$$

The solution of decoherence factor, $f\left(t\right)$, in Born approximation can be solved by taking the inverse Laplace transform of equation 3.3.10

$$f\left(t\right) = f\left(0\right)\left(\cos\left(2\lambda\sqrt{Q_2}t\right) - \frac{iQ_1}{\sqrt{Q_2}}\sin\left(2\lambda\sqrt{Q_2}t\right)\right). \tag{3.3.11}$$

In some physical models, the integration of the intego-differential equation in the Born approximation could not be easily solved and time-local master equations are used to approximate the intego-differential equation. For example, the time-local master equation for our model is obtained by replacing the term $\rho\left(s\right)$ in equation 3.3.6 with $\rho\left(t\right)$ and then the time evolution of the state of the system at time t only depends on the present state $\rho(t)$. Then we get a time-local master equation for our model

$$\dot{\rho}_S(t) = -iTr_B\left[H_I(t), \rho_S(0)\otimes\rho_B\right] - \int_0^t dsTr_B\left\{\left[H_I(t), \left[H_I(s), \rho_S(t)\otimes\rho_B\right]\right]\right\}, \quad (3.3.12)$$

which is called the Redfield equation [61]. The Redfield equation gives the equation of motion for the docoherence factor

$$\dot{f}(t) = -2i\lambda Q_1 f(0) - 4\lambda^2 Q_2 t f(t). \quad (3.3.13)$$

This time-local equation can be easily solved and its solution is

$$f(t) = f(0)\left(\exp\left(-2Q_2\lambda^2t^2\right) - \frac{2i\lambda Q_1}{\exp\left(2\lambda^2Q_2t^2\right)}\int\exp\left(2\lambda^2Q_2t^2\right)dt\right). \quad (3.3.14)$$

b. Born-Markovian approximation

In order to obtain a Markovian master equation from Redfield equation, we need to substitute s by $t-s$ in the integral in equation 3.3.6 and set the upper limit of the integral go to infinity [23, 55]. Then the integrand disappears fast enough for $s \gg \tau_B$. As a result, the Markovian approximation can be made when the bath correlation function decay fast enough that the time scale τ_B over the decay is small compared to the system relaxation time scale τ_S. We obtain the Markovian quantum master equation for our model

$$\dot{\rho}_S(t) = -iTr_B\left[H_I(t-s), \rho_S(0)\otimes\rho_B\right] - \int_0^\infty dsTr_B\left\{\left[H_I(t), \left[H_I(t-s), \rho_S(t)\otimes\rho_B\right]\right]\right\}. \quad (3.3.15)$$

The interaction Hamiltonian in our model is time-independent and we get

$$\dot{\rho}_S(t) = -i\lambda\left[\sigma_z, \rho_S(0)\right] Q_1 - 2\lambda^2\left(\rho_S(t) - \sigma_z \rho_S(t)\sigma_z\right)\int_0^\infty Q_2 ds, \tag{3.3.16}$$

where Q_1 and Q_2 are the expectation value of bath operator J_z and second order bath correlation function, respectively, defined in equation 3.2.11.

In our model, both of the expectation value Q_1 and correlation function Q_2 do not depend on time, which has been discussed in section 3.2. Thus, $\int_0^\infty Q_2 ds$ is infinite. Therefore, the Markovian approximation is not valid for our model. As a result, the dynamics of the reduced density matrix for the central spin is non-Markovian and non-Markovian master equations are expected.

c. The Nakajima-Zwanzig projection operator technique

When an open system S is coupled to an environment B, the dynamics of the density matrix $\rho(t)$ of the total system is specified by

$$H = H_0 + \lambda H_I, \tag{3.3.17}$$

where H_0 is the self Hamiltonian of the system and environment, H_I is the interaction Hamiltonian, and λ is a dimensionless parameter representing the coupling strength. The equation of motion in the interaction picture is

$$\frac{d}{dt}\rho(t) = -i\lambda\left[H_I(t), \rho(t)\right] \equiv \lambda\mathcal{L}(t)\rho(t), \tag{3.3.18}$$

where the interaction Hamiltonian in the interaction picture representation is written as

$$H_I(t) = \exp(iH_0 t) H_I \exp(-iH_0 t). \tag{3.3.19}$$

The *Liouville* super-operator is indicated by $\mathcal{L}(t)$.

A super-operator $\mathcal{P}$ is defined in order to derive an exact equation of motion for the system density matrix ρ_S by

$$\rho \rightarrow \mathcal{P}\rho = \mathrm{Tr}_B\{\rho\} \otimes \rho_B \equiv \rho_S \otimes \rho_B, \tag{3.3.20}$$

where ρ_B is some fixed state of the reservoir. The super-operator $\mathcal{P}$ projects on the relevant part of the total density matrix such that the reduced density matrix ρ_S of the open system can be reconstructed by $\mathcal{P}\rho$. The orthogonal super-operator of $\mathcal{P}$, which projects on the irrelevant part of the density matrix, is denoted by $\mathcal{Q}$,

$$\mathcal{Q}\rho = \rho - \mathcal{P}\rho. \tag{3.3.21}$$

Note that the super-operators $\mathcal{P}$ and $\mathcal{Q}$ are maps in the total Hilbert space $\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_B$ and have properties

$$\begin{aligned} \mathcal{P} + \mathcal{Q} &= I, && (3.3.22)\\ \mathcal{P}^2 &= \mathcal{P}, && (3.3.23)\\ \mathcal{Q}^2 &= \mathcal{Q}, && (3.3.24)\\ \mathcal{P}\mathcal{Q} &= \mathcal{Q}\mathcal{P} = 0, && (3.3.25) \end{aligned}$$

where ρ_B is assumed to be normalized, $Tr_B(\rho_B) = 1$. The density matrix ρ_B defined in equation 3.3.20 is an operator in $\mathcal{H}_B$. It is called the reference state and usually taken to be the Gibbs state of the environment. In may applications, it is usually assumed that the odd moments of the interaction Hamiltonian with respect to the reference state vanish, however, this assumption is not valid for the choice of the reference state in our model.

In order to derive a closed equation for the relevant part $\mathcal{P}\rho\left(t\right)$, we apply the projection operators $\mathcal{P}$ and $\mathcal{Q}$ to the Liouville-von Neumann equation:

$$\frac{\partial}{\partial t}\mathcal{P}\rho\left(t\right)=\mathcal{P}\frac{\partial}{\partial t}\rho\left(t\right)=\lambda\mathcal{P}\mathcal{L}\left(t\right)\rho\left(t\right), \tag{3.3.26}$$

$$\frac{\partial}{\partial t}\mathcal{Q}\rho\left(t\right)=\mathcal{Q}\frac{\partial}{\partial t}\rho\left(t\right)=\lambda\mathcal{Q}\mathcal{L}\left(t\right)\rho\left(t\right). \tag{3.3.27}$$

By inserting the identity $I=\mathcal{P}+\mathcal{Q}$ between the Liouville operator and the density matrix, the above equation set can also be written as

$$\frac{\partial}{\partial t}\mathcal{P}\rho\left(t\right)=\lambda\mathcal{P}\mathcal{L}\left(t\right)\mathcal{P}\rho\left(t\right)+\lambda\mathcal{P}\mathcal{L}\left(t\right)\mathcal{Q}\rho\left(t\right), \tag{3.3.28}$$

$$\frac{\partial}{\partial t}\mathcal{Q}\rho\left(t\right)=\lambda\mathcal{Q}\mathcal{L}\left(t\right)\mathcal{P}\rho\left(t\right)+\lambda\mathcal{Q}\mathcal{L}\left(t\right)\mathcal{Q}\rho\left(t\right). \tag{3.3.29}$$

With a given initial density matrix $\rho\left(t_0\right)$, the solution of equation 3.3.29 can be expressed as

$$\mathcal{Q}\rho\left(t\right)=\mathcal{G}\left(t,t_0\right)\mathcal{Q}\rho\left(t_0\right)+\lambda\int_{t_0}^{t}ds\mathcal{G}\left(t,s\right)\mathcal{Q}\mathcal{L}\left(s\right)\mathcal{P}\rho\left(s\right), \tag{3.3.30}$$

where the propagator

$$\mathcal{G}\left(t,s\right)\equiv T_{\leftarrow}\exp\left[\lambda\int_{s}^{t}ds^{'}\mathcal{Q}\mathcal{L}\left(s^{'}\right)\right]. \tag{3.3.31}$$

The chronological time ordering is described by the operator $T_{\leftarrow}$, which orders any product of super-operators, i.e., the time arguments increase from right to left. The propagator $\mathcal{G}\left(t,s\right)$ satisfies the differential equation

$$\frac{\partial}{\partial t}\mathcal{G}\left(t,s\right)=\lambda\mathcal{Q}\mathcal{L}\left(t\right)\mathcal{G}\left(t,s\right) \tag{3.3.32}$$

with the initial condition

$$\mathcal{G}\left(s,s\right)=I. \tag{3.3.33}$$

The time evolution of the relevant part of the density matrix is obtained by inserting the expression for the irrelevant part of the density matrix 3.3.30 into the equation of motion for the relevant part 3.3.28

$$\begin{aligned}\frac{\partial}{\partial t}\mathcal{P}\rho\left(t\right) &= \lambda\mathcal{P}\mathcal{L}\left(t\right)\mathcal{G}\left(t,t_0\right)\mathcal{Q}\rho\left(t_0\right)+\lambda\mathcal{P}\mathcal{L}\left(t\right)\mathcal{P}\rho\left(t\right)\\ &\quad+\lambda^2\int_{t_0}^{t}ds\mathcal{P}\mathcal{L}\left(t\right)\mathcal{G}\left(t,s\right)\mathcal{Q}\mathcal{L}\left(s\right)\mathcal{P}\rho\left(s\right).\end{aligned} \tag{3.3.34}$$

This is the Nakajima-Zwanzig equation, which is an exact equation of motion for the relevant degrees of freedom of the reduced system. The inhomogeneous term $\lambda\mathcal{P}\mathcal{L}\left(t\right)\mathcal{G}\left(t,t_0\right)\mathcal{Q}\rho\left(t_0\right)$ depends on the initial density matrix and the past history of the system in the time interval $[t_0,t]$. It is vanishes for the factorized initial state $\rho\left(t_0\right)=\rho_S\left(t\right)\otimes\rho_B$ because $\mathcal{P}\rho\left(t_0\right)=\rho\left(t_0\right)$ and $\mathcal{Q}\rho\left(t_0\right)=0$. Then the exact equation for the relevant part of the density matrix is

$$\frac{\partial}{\partial t}\mathcal{P}\rho\left(t\right)=\lambda\mathcal{P}\mathcal{L}\left(t\right)\mathcal{P}\rho\left(t\right)+\int_{t_0}^{t}ds\mathcal{K}\left(t,s\right)\mathcal{P}\rho\left(s\right), \tag{3.3.35}$$

where $\mathcal{K}\left(t,s\right)$ is the memory kernel, a super-operator in the relevant subspace, and reads

$$\mathcal{K}\left(t,s\right)=\lambda^2\mathcal{P}\mathcal{L}\left(t\right)\mathcal{G}\left(t,s\right)\mathcal{Q}\mathcal{L}\left(s\right)\mathcal{P}. \tag{3.3.36}$$

Notice the second term in equation 3.3.35 does not disappear in this model. This is because the condition $Tr_B\left\{H_I\rho_B\left(0\right)\right\}=0$ and $\mathcal{P}\mathcal{L}\left(t\right)\mathcal{P}=0$ do not valid in our model.

Expand the memory kernel in second order, one obtain

$$\mathcal{K}=\lambda^2\mathcal{P}\mathcal{L}\left(t\right)\mathcal{Q}\mathcal{L}\left(s\right)\mathcal{P}+\mathcal{O}\left(\lambda^3\right), \tag{3.3.37}$$

which gives an equation of motion of second order for the relevant part of density matrix

$$\frac{\partial}{\partial t}\mathcal{P}\rho\left(t\right)=\int_{t_0}^{t}ds\lambda^2\mathcal{P}\mathcal{L}\left(t\right)\mathcal{Q}\mathcal{L}\left(s\right)\mathcal{P}\rho\left(s\right)+\lambda\mathcal{P}\mathcal{L}\left(t\right)\mathcal{P}\rho\left(t\right) \tag{3.3.38}$$

We can get the Nakajima-Zwanzig projection operator equation in second order by introducing the expression for the projection operator $\mathcal{P}$ and for the generator $\mathcal{L}\left(t\right)$

$$\frac{\partial}{\partial t}\rho_S\left(t\right)=-\lambda^2\int_{0}^{t}dsTr_B\left[H_I\left(t\right),\left[H_I\left(s\right),\rho_S\left(s\right)\otimes\rho_B\right]\right]-i\lambda Tr_B\left[H_I\left(t\right),\rho_S\left(t\right)\otimes\rho_B\right]. \tag{3.3.39}$$

d. Time-Convolutionless master equation

Because the Nakajima-Zwanzig equation has the time convolution in the memory kernel, the equation of motion for the reduced system is difficult to treat. The time-convolutionless projection operator method is introduced and the dependence of the future time evolution on the history of the system is removed in the master equation. It is achieved by replacing the density matrix $\rho\left(s\right)$ on the right-hand side of equation 3.3.30 by

$$\rho\left(s\right)=G\left(t,s\right)\left(\mathcal{P}+\mathcal{Q}\right)\rho\left(t\right), \tag{3.3.40}$$

where $G\left(t,s\right)$ is the backward propagator, which the inverse of the unitary time evolution, of the whole system. It reads

$$G\left(t,s\right)=T_{\rightarrow}\exp\left[-\lambda\int_{s}^{t}ds^{'}\mathcal{L}\left(s^{'}\right)\right], \tag{3.3.41}$$

where $T_{\rightarrow}$ denotes the anti-chronological time-ordering.

The irrelevant part of the density matrix can be written as

$$\mathcal{Q}\rho(t) = \mathcal{G}(t,t_0)\,\mathcal{Q}\rho(t_0) + \lambda\int_{t_0}^{t} ds\mathcal{G}(t,s)\,\mathcal{Q}\mathcal{L}(s)\,\mathcal{P}G(t,s)\,(\mathcal{P}+\mathcal{Q})\,\rho(t)\,. \tag{3.3.42}$$

By introducing the super-operator

$$\Sigma(t) = \lambda\int_{t_0}^{t} ds\mathcal{G}(t,s)\,\mathcal{Q}\mathcal{L}(s)\,\mathcal{P}G(t,s)\,, \tag{3.3.43}$$

the irrelevant part of the density matrix can be expressed as

$$[1-\Sigma(t)]\,\mathcal{Q}\rho(t) = \mathcal{G}(t,t_0)\,\mathcal{Q}\rho(t_0) + \Sigma(t)\,\mathcal{P}\rho(t)\,. \tag{3.3.44}$$

Because $\Sigma(t)$ has the properties $\Sigma(t)\,|_{\alpha=0} = 0$ and $\Sigma(t_0) = 0$, the term $1-\Sigma(t)$ could be inverted for small couplings and any situation for small $t-t_0$. Then

$$\mathcal{Q}\rho(t) = [1-\Sigma(t)]^{-1}\,\Sigma(t)\,\mathcal{P}\rho(t) + [1-\Sigma(t)]^{-1}\,\mathcal{G}(t-t_0)\,\mathcal{Q}\rho(t_0)\,. \tag{3.3.45}$$

One can read the information that the irrelevant part $\mathcal{Q}\rho(t)$ of the density matrix can be determined by the relevant part $\mathcal{P}\rho(t)$ at time t and the initial state $\mathcal{Q}\rho(t_0)$. By introducing the exact backward propagator $G(t,s)$, the history dependence of the relevant part in the Nakajima-Zwanzig equation is removed in the time-convolutionless approach. Insert the equation of irrelevant part into the equation of motion for the relevant part, we can derive the exact time-convolutionless (TCL) equation

$$\frac{\partial}{\partial t}\mathcal{P}\rho(t) = \mathcal{K}(t)\,\mathcal{P}\rho(t) + \mathcal{I}(t)\,\mathcal{Q}\rho(t_0)\,, \tag{3.3.46}$$

where $\mathcal{K}(t)$ is the TCL generator, which is a time-local generator, and reads

$$\mathcal{K}(t) = \lambda\mathcal{P}\mathcal{L}(t)\,[1-\Sigma(t)]^{-1}\,\mathcal{P}. \tag{3.3.47}$$

The term $\mathcal{I}(t)$ is the inhomogeneity

$$\mathcal{I}(t) = \lambda \mathcal{P}\mathcal{L}(t) \left[1 - \Sigma(t)\right]^{-1} \mathcal{G}(t, t_0) \mathcal{Q}, \tag{3.3.48}$$

which vanishes for the factorized initial condition $\rho(t_0) = \rho_S(t) \otimes \rho_B$. The exact time-convolutionless equation for the factorized initial condition is

$$\frac{\partial}{\partial t} \mathcal{P}\rho(t) = \mathcal{K}(t) \mathcal{P}\rho(t).$$

The super-operator $\mathcal{K}(t)$ only exists when one can invert the operator $\left[1 - \Sigma(t)\right]^{-1}$. Assume $\Sigma(t)$ can be expanded as

$$\left[1 - \Sigma(t)\right]^{-1} = \sum_{n=0}^{\infty} \left[\Sigma(t)\right]^n. \tag{3.3.49}$$

By substituting above expression into equation 3.3.47, we have

$$\mathcal{K}(t) = \lambda \sum_{n=0}^{\infty} \mathcal{P}\mathcal{L}(t) \left[\Sigma(t)\right]^n \mathcal{P} = \sum_{n=1}^{\infty} \lambda^n \mathcal{K}_n(t). \tag{3.3.50}$$

In order to determine $\mathcal{K}_n(t)$, we expand $\Sigma(t)$ in powers of λ.

$$\Sigma(t) = \sum_{n=1}^{\infty} \lambda^n \Sigma_n(t). \tag{3.3.51}$$

On substituting above equation into equation 3.3.50, we get $\mathcal{K}_n(t)$. Here, we use the first four terms of the expansion derived in Ref [23]:

$$\mathcal{K}_1(t) = \mathcal{P}\mathcal{L}(t) \mathcal{P}, \tag{3.3.52}$$

$$\mathcal{K}_2\left(t\right)=\int_0^t dt_1 \mathcal{P}\mathcal{L}\left(t\right)\mathcal{L}\left(t_1\right)\mathcal{P}, \tag{3.3.53}$$

$$\mathcal{K}_3\left(t\right)=\int_0^t dt_1\int_0^{t_1} dt_2 \mathcal{P}\mathcal{L}\left(t\right)\mathcal{L}\left(t_1\right)\mathcal{L}\left(t_2\right)\mathcal{P}, \tag{3.3.54}$$

$$\begin{aligned}\mathcal{K}_4\left(t\right)=&\int_0^t dt_1\int_0^{t_1} dt_2\int_0^{t_2} dt_3 (\mathcal{P}\mathcal{L}\left(t\right)\mathcal{L}\left(t_1\right)\mathcal{L}\left(t_2\right)\mathcal{L}\left(t_3\right)\mathcal{P}-\mathcal{P}\mathcal{L}\left(t\right)\mathcal{L}\left(t_1\right)\mathcal{P}\mathcal{L}\left(t_2\right)\mathcal{L}\left(t_3\right)\mathcal{P}\\ &-\mathcal{P}\mathcal{L}\left(t\right)\mathcal{L}\left(t_2\right)\mathcal{P}\mathcal{L}\left(t_1\right)\mathcal{L}\left(t_3\right)\mathcal{P}-\mathcal{P}\mathcal{L}\left(t\right)\mathcal{L}\left(t_3\right)\mathcal{P}\mathcal{L}\left(t_1\right)\mathcal{L}\left(t_2\right)\mathcal{P}).\end{aligned} \tag{3.3.55}$$

The corresponding terms for our model are obtained by introducing the expression for the projection operator $\mathcal{P}$ and for the generator $\mathcal{L}\left(t\right)$

$$\mathcal{K}_1\left(t\right)\mathcal{P}\rho\left(t\right)=-i\lambda Tr_B\left\{\left[H_I,\rho_S\left(t\right)\otimes\rho_B\right]\right\}\otimes\rho_B, \tag{3.3.56}$$

$$\mathcal{K}_2\left(t\right)\mathcal{P}\rho\left(t\right)=-\lambda^2 t Tr_B\left\{\left[H_I,\left[H_I,\rho_S\left(t\right)\otimes\rho_B\right]\right]\right\}\otimes\rho_B, \tag{3.3.57}$$

$$\mathcal{K}_3\left(t\right)\mathcal{P}\rho\left(t\right)=i\lambda^3\frac{t^2}{2}Tr_B\left\{\left[H_I,\left[H_I,\left[H_I,\rho_S\left(t\right)\otimes\rho_B\right]\right]\right]\right\}\otimes\rho_B, \tag{3.3.58}$$

$$\begin{aligned}\mathcal{K}_4\left(t\right)\mathcal{P}\rho\left(t\right) \;=\;& \lambda^4\frac{t^3}{6}(Tr_B\left\{\left[H_I,\left[H_I,\left[H_I,\left[H_I,\rho_S\left(t\right)\otimes\rho_B\right]\right]\right]\right]\right\}\otimes\rho_B\\ &-3Tr_B\left\{\left[H_I,\left[H_I,Tr_B\left\{\left[H_I,\left[H_I,\rho_S\left(t\right)\otimes\rho_B\right]\right]\right\}\otimes\rho_B\right]\right]\right\}\otimes\rho_B)\end{aligned} \tag{3.3.59}$$

The second-order, third-order, and fourth-order TCL equation for the reduced density matrix $\rho_S\left(t\right)$ are

$$\frac{\partial}{\partial t}\rho_S(t) = -i\lambda Q_1\left[\sigma_z, \rho_S(t)\right] - 2\lambda^2 t Q_2\left(\rho_S(t) - \sigma_z \rho_S(t)\sigma_z\right), \tag{3.3.60}$$

$$\begin{aligned} \frac{\partial}{\partial t}\rho_S(t) &= -i\lambda Q_1\left[\sigma_z, \rho_S(t)\right] - 2\lambda^2 t Q_2\left(\rho_S(t) - \sigma_z \rho_S(t)\sigma_z\right) \\ &\quad + 4i\lambda^3 Q_3 \frac{t^2}{2}\left(\sigma_z \rho_S(t) - \rho_S(t)\sigma_z\right), \end{aligned} \tag{3.3.61}$$

$$\begin{aligned} \frac{\partial}{\partial t}\rho_S(t) &= -i\lambda Q_1\left[\sigma_z, \rho_S(t)\right] - 2\lambda^2 t Q_2\left(\rho_S(t) - \sigma_z \rho_S(t)\sigma_z\right) \\ &\quad + 2i\lambda^3 t^2 Q_3\left(\sigma_z \rho_S(t) - \rho_S(t)\sigma_z\right) \\ &\quad + \lambda^4 \frac{t^3}{6}\left(8Q_4 - 24Q_2^2\right)\left(\rho_S(t) - \sigma_z \rho_S(t)\sigma_z\right). \end{aligned} \tag{3.3.62}$$

The corresponding decoherence factor, $f(t)$, can be solved analytically by using these equations:

$$f_{TCL2}(t) = \exp\left(-2i\lambda Q_1 t - 2\lambda^2 t^2 Q_2\right), \tag{3.3.63}$$

$$f_{TCL3}(t) = \exp\left(-2i\lambda Q_1 t - 2\lambda^2 t^2 Q_2 + i\lambda^3 Q_3 \frac{4}{3} t^3\right), \tag{3.3.64}$$

$$f_{TCL4}(t) = \exp\left(-2iQ_1\lambda t - 2Q_2\lambda^2 t^2 + i\frac{4}{3}Q_3\lambda^3 t^3 + \left(\frac{2}{3}Q_4 - 2Q_2^2\right)\lambda^4 t^4\right), \tag{3.3.65}$$

where Q_1, Q_2, Q_3 and Q_4 are defined by 3.2.11.

3.4 Plots and comparisons

In this section exact and approximation solutions are plotted for various parameters, and the performances of different approximation techniques can be discussed by comparing them with exact solutions. In the following figures, all the dynamics are plotted in terms of the dimensionless parameter λt.

3.5.1 Exact Solution

For all of the three initial bath states situations introduced in section 3.2, we consider the exact solutions of the reduced system density matrix for three different numbers of bath spins, $N = 10$, 20, and 100. For the spin bath is initially in a thermal equilibrium state at a finite temperature situation, three different temperatures, $\beta = 0.001$, 0.5, and 3 are considered. Figure 3.4.1 and 3.4.2 show the plots for the exact solutions of $\mathrm{Re}\left(f\left(t\right)\right)$ and $\left|f\left(t\right)\right|$, respectively, with spin bath is initially in thermal equilibrium at finite temperature introduced in part (a) of section 3.2.1 and $\beta = 0.001$. For each figure, exact solutions for $N = 10$, 20, and 100 are plotted. Figure 3.4.3 and 3.4.4 show the plots for the exact solutions of $\mathrm{Re}\left(f\left(t\right)\right)$ and $\left|f\left(t\right)\right|$, respectively, with spin bath is initially in thermal equilibrium at a finite temperature and $\beta = 0.5$. For each figure, exact solutions for $N = 10$, 20, and 100 are plotted. Figure 3.4.5 and 3.4.6 show the plots for the exact solutions of $\mathrm{Re}\left(f\left(t\right)\right)$ and $\left|f\left(t\right)\right|$, respectively, with spin bath is initially in thermal equilibrium at a finite temperature and $\beta = 3$. For each figure, exact solutions for $N = 10$, 20, and 100 are plotted.Figure 3.4.7 and 3.4.8 show the exact solution for $\mathrm{Re}\left(f\left(t\right)\right)$ and $\left|f\left(t\right)\right|$, respectively, with spin bath is initially at an polarized state, which is the infinitely high temperature case, introduced in part (b) of section 3.2.1. For each figure, exact solutions for $N = 10$, 20, and 100 are plotted. Figure 3.4.9 shows the exact solutions for $\mathrm{Re}\left(f\left(t\right)\right)$ and $\left|f\left(t\right)\right|$ with the spin bath is initially in its ground state, which is introduced in part (c) of section 3.2.1. For each figure, exact solutions for $N = 10$, 20, and 100 are plotted.

As can be seen, for all the parameters we have chosen, the evolutions of $\mathrm{Re}\left(f\left(t\right)\right)$ and $\left|f\left(t\right)\right|$ always return to their initial value, 1, at a fix time. As the time t is expressed in terms of λ

in the plots, we can conclude that the full recurrence time for the decoherence factor in our model is determined by the coupling strength between the central spin and the spin bath. This result is consistent with the discussions about equation 3.2.9 in section 3.2.

Figure 3.4.1 shows that there is no partial recurrence for $\mathrm{Re}\,(t)$ when the spin bath is initially in a thermal state at high temperature $(\beta = 0.001)$. When the temperature decreases $(\beta = 0.5)$, it can be seen from Figure 3.4.3 that $\mathrm{Re}\,(t)$ starts to have partial recurrences. And Figure 3.4.5 shows that $\mathrm{Re}\,(f\,(t))$ has collapse and revival at low temperature $(\beta = 3)$. This is because at a very high temperature, the density matrix for the spin bath is an unpolarized state such that the population weight in each eigenstate $|\lambda, j, m\rangle$ is the same. These results are further confirmed by Figure 3.4.7 and 3.4.9, which plot $\mathrm{Re}\,(f\,(t))$ for infinite high temperature situation and ground state situation.

All the plots show that the increase of the number of spins N in the spin bath will not affect the period for the full recurrences, but will accelerate the evolution of the decoherence factor. It can be seen from Figure 3.4.1 and 3.4.2, the decoherence factor with a larger spin number in the spin bath goes to 0 much faster than it with a smaller number. And for the low temperature $(\beta = 3)$ case shown in figure 3.4.5 and 3.4.6, the increase of the spin numbers will also increase the number of partial recurrences in a period of full recurrence.

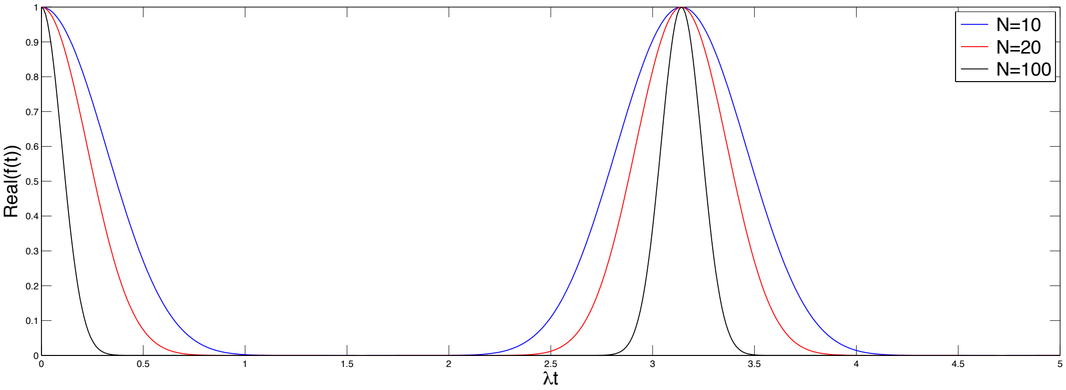

Figure 3.4.1: Comparison of the exact solutions for $\mathrm{Re}\,(f\,(t))$ at $\beta = 0.001$ with initial state of spin bath is at thermal equilibrium for $N = 10$, 30, and 100.

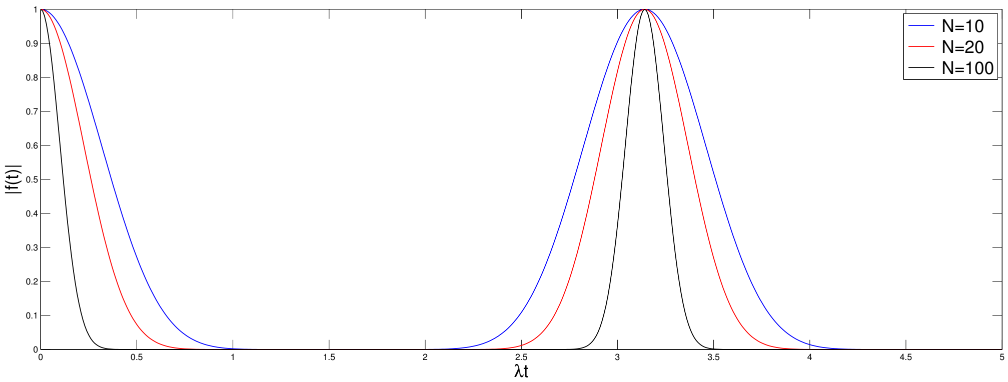

Figure 3.4.2: Comparison of the exact solutions for $|f(t)|$ at $\beta = 0.001$ with initial state of spin bath is at thermal equilibrium for $N = 10$, 30, and 100.

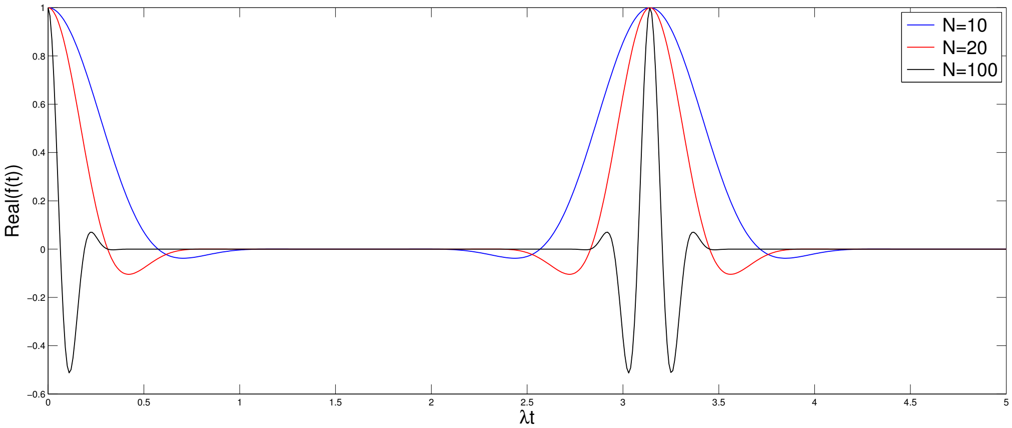

Figure 3.4.3: Comparison of the exact solutions for $\mathrm{Re}(f(t))$ at $\beta = 0.5$ with initial state of spin bath is at thermal equilibrium for $N = 10$, 30, and 100.

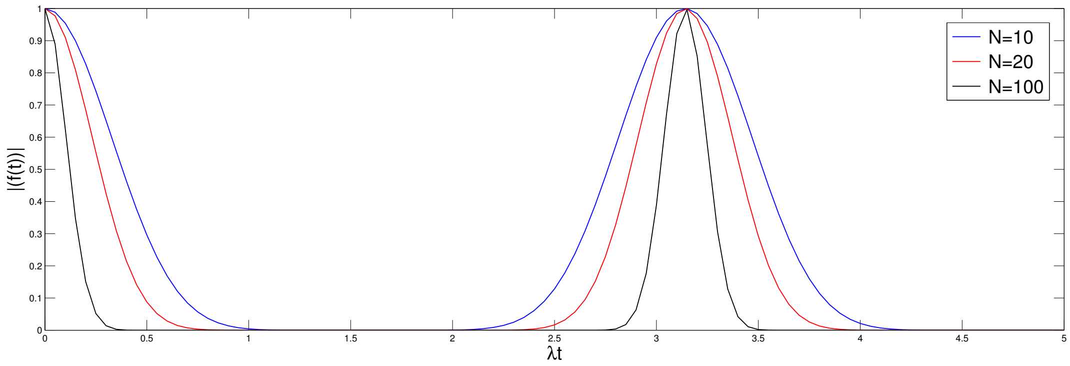

Figure 3.4.4: Comparison of the exact solutions for $|f(t)|$ at $\beta = 0.5$ with initial state of spin bath is at thermal equilibrium for $N = 10$, 30, and 100.

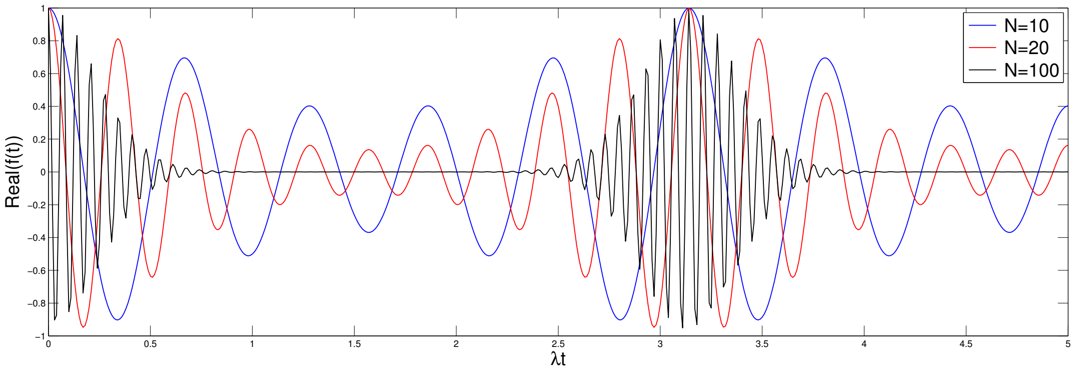

Figure 3.4.5: Comparison of the exact solutions for $\mathrm{Re}(f(t))|$ at $\beta = 3$ with initial state of spin bath is at thermal equilibrium for $N = 10$, 30, and 100.

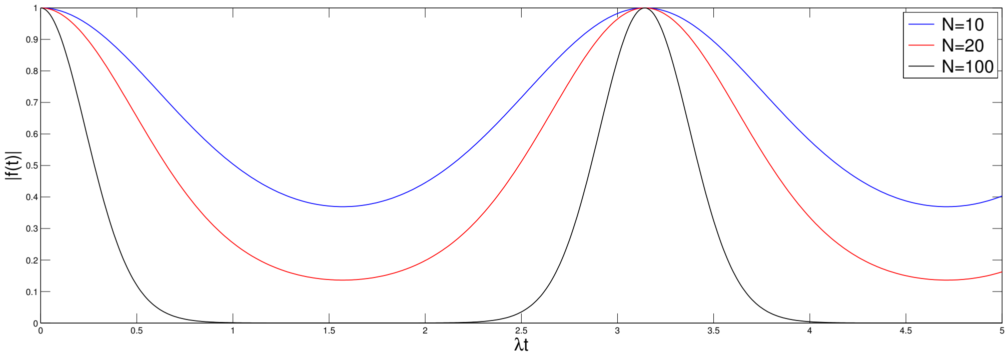

Figure 3.4.6: Comparison of the exact solutions for $|f(t)|$ at $\beta = 3$ with initial state of spin bath is at thermal equilibrium for $N = 10$, 30, and 100.

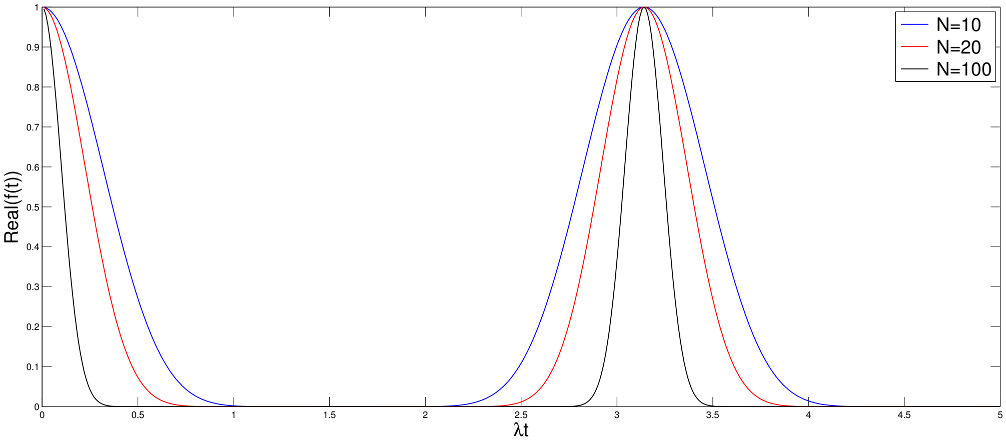

Figure 3.4.7: Comparison of the exact solutions for $\mathrm{Re}(f(t))$ with initial state of spin bath is an unpolarized state for $N = 10$, 30, and 100.

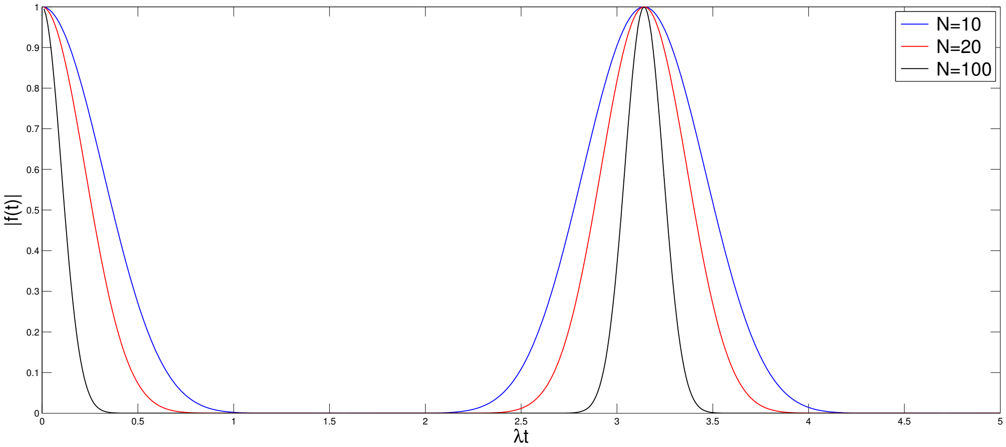

Figure 3.4.8: Comparison of the exact solutions for $|f(t)|$ with initial state of spin bath is an unpolarized state for $N = 10$, 30, and 100.

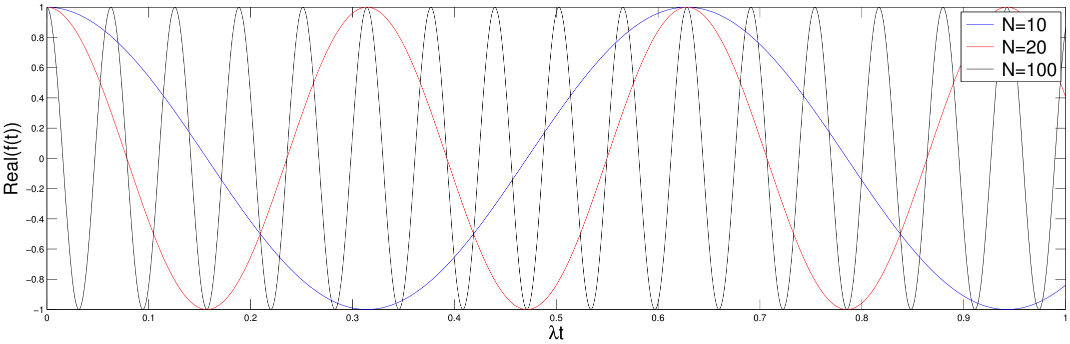

Figure 3.4.9: Comparison of the exact solution for $\mathrm{Re}(f(t))$ with initial state of spin bath is in its ground state for $N = 10$, 30, and 100.

3.5.2 Comparison of approximation solutions with the exact solution

Firstly, we compare the exact solutions of $\mathrm{Re}(f(t))$ with NZ2 and TCL2 approximation solutions for various parameters. Figure 3.4.10 shows the comparison of the exact solution with NZ2 and TCL2 solutions for $\mathrm{Re}(f(t))$ with $\beta = 0.001$ and $N = 10$. Figure 3.4.11

shows the comparison of the exact solution with NZ2 and TCL2 solutions for $\mathrm{Re}\left(f\left(t\right)\right)$ with $\beta = 3$ and $N = 10$. As can be seen, when the spin number is small ($N = 10$), NZ2 and TCL2 approximate the short-time behavior of exact solutions well for both high ($\beta = 0.001$) and low ($\beta = 3$) temperature well. However, Figure 3.4.10 shows that at high temperature ($\beta = 0.001$), NZ2 diverges from the exact solution after a short time period of time while TCL2 fits the exact solution well during the time period we plotted. Figure 3.4.11 shows that at low temperature $\left(\beta = 3\right)$, TCL2 diverges from the exact solution after a short period of time while NZ2 fits the exact solution well during the time period we plotted.

Figure 3.4.12 shows the comparison of the exact solution with NZ2 and TCL2 solutions for $\mathrm{Re}\left(f\left(t\right)\right)$ with $\beta = 0.001$ and $N = 100$. Figure 3.4.13 shows the comparison of the exact solution with NZ2 and TCL2 solutions for $\mathrm{Re}\left(f\left(t\right)\right)$ with $\beta = 3$ and $N = 100$. As can be seen, when the spin number is large ($N = 100$), NZ2 and TCL2 approximate the short-time behavior of exact solutions well for both high ($\beta = 0.001$) and low ($\beta = 3$) temperature well. However, Figure 3.4.12 shows that at high temperature ($\beta = 0.001$), NZ2 diverges from the exact solution after a short time period of time while TCL2 fits the exact solution well during the time period we plotted. Figure 3.4.13 shows that at low temperature $\left(\beta = 3\right)$, TCL2 diverges from the exact solution after a short period of time while NZ2 fits the exact solution well during the time period we plotted.

As a result, the number of spins in the spin bath does not affect the performances of NZ2 and TCL2; however, the temperature for the initial state of the spin bath does. For our model, TCL2 approximates the exact solution better than NZ2 at a high temperature ($\beta = 0.001$) and NZ2 approximates the exact solution better than TCL2 at low temperature ($\beta = 3$).

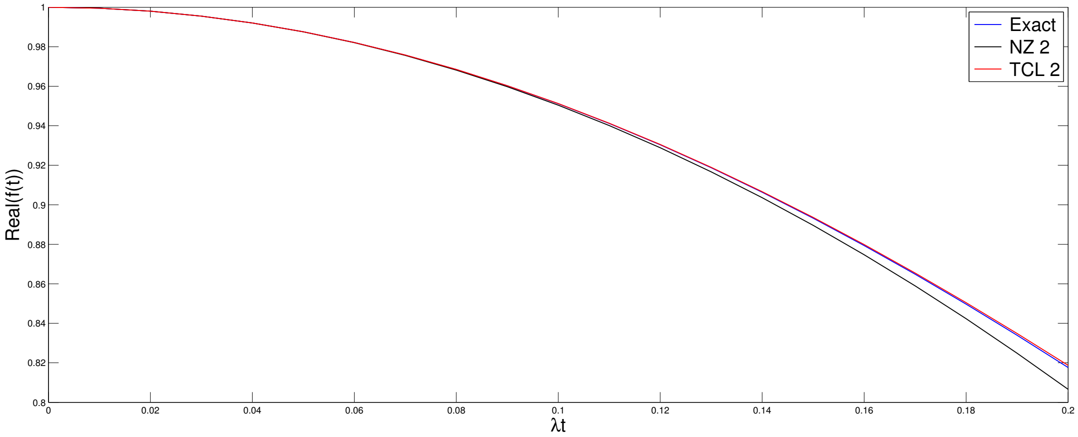

Figure 3.4.10: Comparison of the exact solution with NZ2 and TCL2 solutions for $\mathrm{Re}\left(f\left(t\right)\right)$ with $\beta = 0.001$ and $N = 10$.

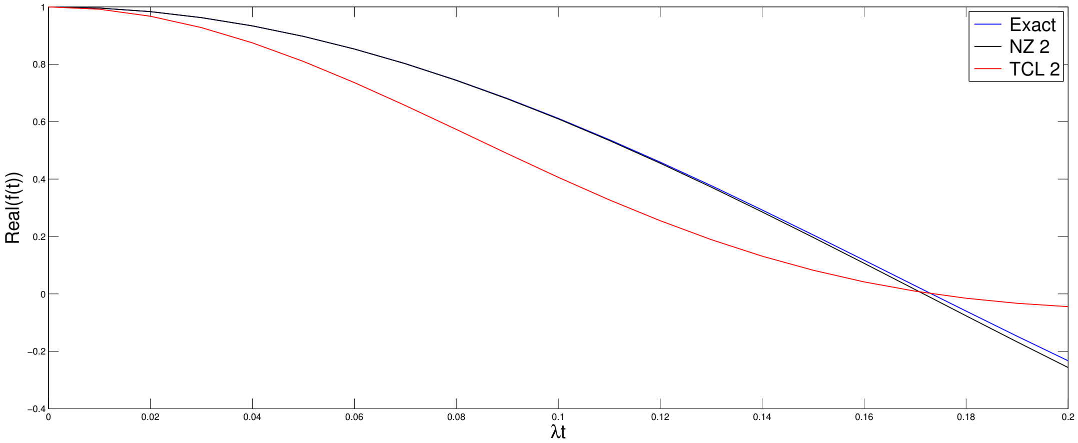

Figure 3.4.11: Comparison of the exact solution with NZ2 and TCL2 solutions for $\mathrm{Re}\left(f\left(t\right)\right)$ with $\beta = 3$ and $N = 10$.

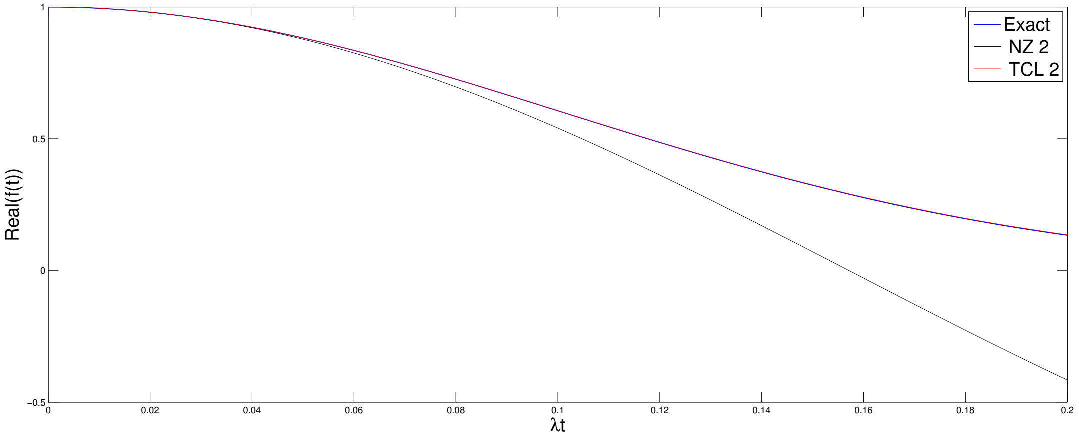

Figure 3.4.12: Comparison of the exact solution with NZ2 and TCL2 solutions for $\mathrm{Re}\left(f\left(t\right)\right)$ with $\beta = 0.001$ and $N = 100$.

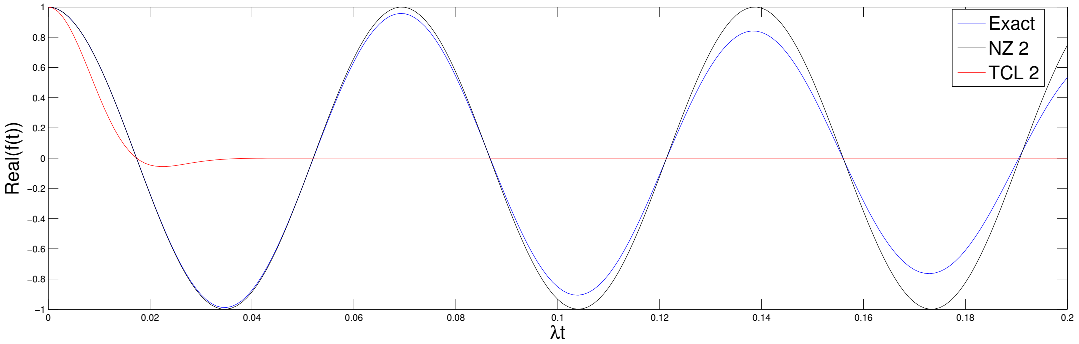

Figure 3.4.13: Comparison of the exact solution with NZ2 and TCL2 solutions for $\mathrm{Re}\left(f\left(t\right)\right)$ with $\beta = 3$ and $N = 100$.

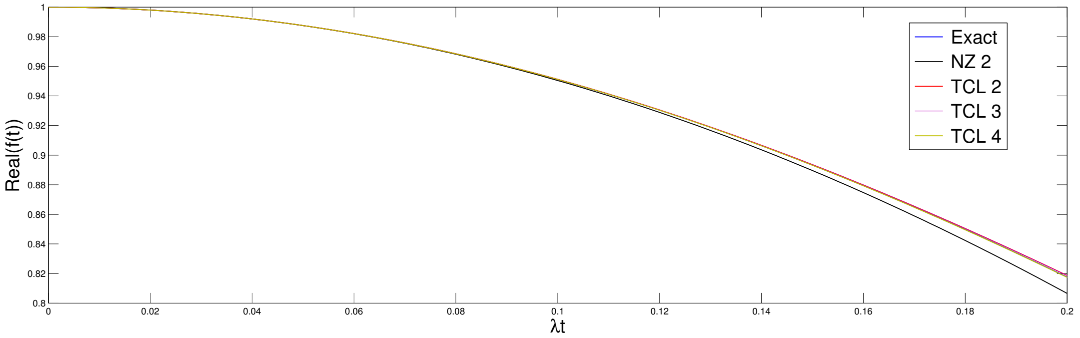

Figure 3.4.14: Comparison of the exact solution with NZ2, TCL2, TCL3, and TCL4 solutions for $\mathrm{Re}\left(f\left(t\right)\right)$ with $\beta = 0.001$ and $N = 10$.

3.5 Chapter Discussion

In this Chapter we have discussed the exact solutions, the performances of two different projection operators, Nakajima-Zwanzig (NZ) and Time-convolutionless (TCL), for an exactly solvable spin-star model. The structure of the model is the same as the model introduced in Ref [25], but with different interaction Hamiltonian: a central spin is interacting with a bath of spins through an Ising coupling, which leads to the pure dephasing of the qubit. In Ref [26] the same model with same interaction Hamiltonian has been studied, however, we focus on the approaches by using the collective operator methods. This pure dephasing model can be solved exactly due to its high symmetry structure. As a result, we can compare the performances of NZ and TCL methods with the exact solution directly. The Born approximation for this model is also studied, however the Born-Markovian approximation is shown to be not applicable in this model. This is mainly because the time-independent bath correlation functions. Therefore, the dynamics of the central spin is non-Markovian.

As pointed in Ref [51], the performances of the perturbation techniques of the decoherence factor can strongly depend on the specific properties of the model, e.g., the interaction Hamiltonian, the initial state of the spin environment, and the bath spectral density.

For our model, the TCL expansion to second order gives a more accurate answer than the second order NZ expansion at a high temperature ($\beta = 0.001$) . However, the second order NZ expansion turns out to be more accurate than the second order TCL expansion at low temperature ($\beta = 3$). This can be clarified by considering the Taylor expansion of the decoherence factor $f\left(t\right)$:

$$f\left(t\right) = 1 - 2i\lambda t Q_1 - 2\lambda^2 t^2 Q_2 + \frac{4}{3} i\lambda^3 t^3 Q_3 + \frac{2}{3}\lambda^4 t^4 Q_4 + \ldots, \tag{3.5.1}$$

and

$$\mathrm{Re}\left(f\left(t\right)\right) = 1 - 2Q_2\left(\lambda t\right)^2 + \frac{2}{3}Q_4\left(\lambda t\right)^4 + \mathcal{O}\left(\left(\lambda t\right)^6\right). \tag{3.5.2}$$

The corresponding expansion obtained from TCL2 is given by

$$\mathrm{Re}\left(f\left(t\right)\right) = 1 - 2\left(Q_2 + Q_1^2\right)\left(\lambda t\right)^2 + \left(2Q_2^4 - 4Q_1^2 Q_2 + \frac{2}{3}Q_1^4\right)\left(\lambda t\right)^4 + \mathcal{O}\left(\left(\lambda t\right)^6\right), \tag{3.5.3}$$

and NZ2 is given by

$$\mathrm{Re}\left(f\left(t\right)\right) = 1 - 2Q_2\left(\lambda t\right)^2 + \frac{2}{3}Q_2\left(\lambda t\right)^4 + \mathcal{O}\left(\left(\lambda t\right)^6\right). \tag{3.5.4}$$

At the high temperature, $\beta = 0.001$, the first order correlation function of bath, Q_1, is a very small value and can be neglect. In this situation, the second order coefficients for NZ2 and TCL2 are both same as the exact solution, however, neither NZ2 or TCL2 give the correct fourth order coefficients. The fourth order coefficient for TCL2 is closer to the exact fourth order coefficient at medium and high temperature. In contrast, the fourth order coefficient for

NZ2 is more accurate at low temperature. Therefore, our model demonstrate the situations where TCL2 works better and NZ2 works better.

As a result, the specific properties of open quantum systems should be considered when the applications of the projection operator methods are performed.

Chapter 4

Outlook: The Open Spin-Star Model

In this chapter we discuss the time evolution of the reduced density matrix for a central spin (qubit) subjected to the spin-star system, which is again coupled to a thermal bath (a set of Harmonic oscillators). This nonlinear environment is non-Gaussian and non-Markovian. We assume the coupling between the qubit and the spin-star system is weak such that the spin-star system and the Harmonic oscillator bath together can be approximated as a Gaussian environment. Therefore, we could calculate the reduced density matrix elements by using the bath correlation function, which is obtained by using quantum regression theorem. Similar problems have been studied in Ref [62, 63, 64, 65, 66].

4.1 The nonlinear model

In this thesis, we mainly focus on the study of the non-Gaussian pure dephasing model and therefore the interaction between the qubit and its whole environment is of form:

$$H_I = \lambda \sigma_z \otimes J_z \otimes I_B, \tag{4.1.1}$$

where λ is the coupling strength between the qubit and the spin-star system, σ_z is the Pauli matrix for the qubit, J_z is the collective operator for the spin-star system, and I_B is the identity operator in the Hilbert space of the Harmonic oscillator bath. This coupling Hamiltonian can be simply written as $\lambda \sigma_z \otimes J_z$.

In our model, the interaction Hamiltonian between the spin-star system and the Harmonic oscillator bath reads

$$H_I' = I_q \otimes J_x \otimes \sum_i g_i \left(a_i^\dagger + a_i \right), \tag{4.1.2}$$

where I_q is the identity operator in the Hilbert space of the qubit, J_x is the collective operator of spin bath defined in Chapter 3, $a_i^\dagger$ and a_i are creation and annihilation operators for the heat reservoir, and g_i is the coupling strength between the pseudo-large spin and ith boson in the heat reservoir.

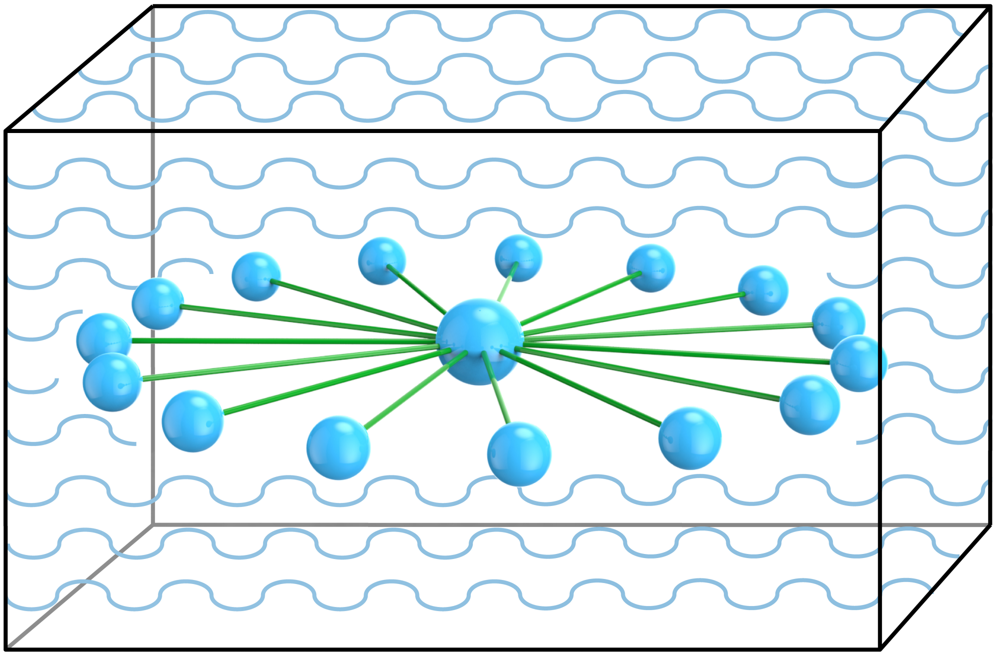

Figure 4.1.1: The diagram of the open spin-star configuration consisting a single central spin-$\frac{1}{2}$ system equally coupled with N spin-$\frac{1}{2}$ in the spin bath, which is again couple to a thermal bath. The spins in the bath are not coupled to one another.

Then the Hamiltonian of the whole system is

$$H = \frac{\omega_0}{2}\sigma_z + \lambda\sigma_z \otimes J_z + \Omega J_z + J_x \otimes \sum_i g_i \left(a_i^\dagger + a_i\right) + \sum_i \omega_i a_i^\dagger a_i, \tag{4.1.3}$$

where ω_0 is the energy splitting of the central spin and Ω is the energy splitting of the spin in the spin bath.

The environment Hamiltonian of the qubit is

$$H_B = \Omega J_z + J_x \otimes \sum_i g_i \left(a_i^\dagger + a_i\right) + \sum_i \omega_i a_i^\dagger a_i. \tag{4.1.4}$$

We are interested in the reduced dynamics of the central spin (qubit), which is obtained from tracing out all the degrees of freedom of the environment:

$$\begin{aligned}
\langle 0|\rho_q(t)|1\rangle &= \langle 0|Tr_B\left\{e^{-iHt}\rho(0)\,e^{iHt}\right\}|1\rangle \\
&= \langle 0|Tr_B\left\{e^{-i\left(\frac{\omega_0}{2}\sigma_z+\lambda\sigma_z\otimes J_z+H_B\right)t}\rho_q(0)\otimes\rho_B(0)\,e^{+i\left(\frac{\omega_0}{2}\sigma_z+\lambda\sigma_z\otimes J_z+H_B\right)t}\right\}|1\rangle \\
&= \langle 0|\rho_q(0)|1\rangle\cdot e^{-i\omega_0 t}\cdot Tr_B\left\{e^{-i(\lambda J_z+H_B)t}\rho_B(0)\,e^{+i(-\lambda J_z+H_B)t}\right\} \\
&= \langle 0|\rho_q(0)|1\rangle\cdot e^{-i\omega_0 t}\cdot f(t),
\end{aligned} \tag{4.1.5}$$

where $f(t) = \langle e^{-i(\lambda J_z+H_B)t}e^{+i(-\lambda J_z+H_B)t}\rangle$.

Because the exact solution of $f(t)$ could not be easily obtained for large N, we apply Gaussian approximation to the environment of the central spin (qubit). As a result, the decoherence factor $f(t)$ can be obtained by using the two-time environment correlation function $\langle J_z(t+\tau)\,J_z(\tau)\rangle$, see Chapter 2.

4.2 Calculation of the open spin-star system correlation function

We start with the full Hamiltonian of the Gaussian environment:

$$\hat{H}_B = \Omega \hat{J}_z + \hat{J}_x \otimes \sum_i \lambda_i \left(\hat{a}_i^\dagger + \hat{a}_i \right) + \sum_i \omega_i \hat{a}_i^\dagger \hat{a}_i, \tag{4.2.1}$$

Notice that if we make rotating-wave approximation (RWA), i.e. ignore the terms $J_+ a_i$ and $J_- a_i^+$ which correspond to simultaneous creation of a photon and atomic excitation, then above equation becomes to

$$H_B = \Omega J_z + \sum_i \omega_i \hat{a}_i^+ \hat{a}_i + \sum_i \left(\lambda_i J_- \hat{a}_i^+ + \lambda_i J_+ \hat{a}_i \right) \tag{4.2.2}$$

In this thesis, we consider the weak coupling regime and derive a Lindblad master equation in Born, Markov, and secular (BMS) approximation describing the time evolution of the large spin system.

$$\begin{aligned} \frac{d}{dt}\rho_S(t) = &-i\left[\Omega J_z, \rho_S(t)\right] + \gamma(\bar{n}+1)\left(2J_-\rho_S(t)J_+ - J_+J_-\rho_S(t) - \rho_S(t)J_+J_-\right) \\ &+ \gamma\bar{n}\left(2J_+\rho_S(t)J_- - J_-J_+\rho_S(t) - \rho_S(t)J_-J_+\right). \end{aligned} \tag{4.2.3}$$

This is the master equation for the reduced density matrix of the spin-star system. When $\bar{n} = 0$, it can be solved analytically [54]. In this thesis, we assume the temperature of the heat bath is low and $\bar{n} \approx 0$. This master equation becomes

$$\frac{d}{dt}\rho_S(t) = -i\left[\Omega J_z, \rho_S(t)\right] + \gamma\left(2J_-\rho_S(t)J_+ - J_+J_-\rho_S(t) - \rho_S(t)J_+J_-\right) \tag{4.2.4}$$

We solve it by the method of eigenvectors expansion. The collective operators J_z, J_+, and J_- are defined in chapter 3 by equations 3.1.7, 3.1.9, and 3.1.10, respectively. By observing the master equation, the operators J_z , J_-, and J_+ only generate rates for density matrix with same j value and only density matrix elements with same j value are involved in the same master equation. When the initial density matrix of spin-star system is diagonal, this master equation will not generate undiagonal elements. For the sake of simplicity, we denote the element of the reduced density matrix for the spin-star system $\langle\lambda, j, m|\rho_S\left(t\right)|\lambda, j, m\rangle$ as $\rho_{j,mm}\left(t\right)$, which has enough information for the analysis in this thesis.

In order to solve 4.2.4 by the method of eigenvectors expansion, we take it's elements in the eigenstates $|\lambda, j, m\rangle$:

$$\frac{d}{dt}\rho_{j,m}\left(t\right) = \gamma C_{j,m+}^2\rho_{j,m+1}\left(t\right) - \gamma\left(C_{j,m-}^2 + C_{j,m+}^2\right)\rho_{j,m}\left(t\right), \tag{4.2.5}$$

where we have defined the eigenvalues of J_+ and J_- in the eigenstate $|\lambda, j, m\rangle$ as

$$C_{j,m+} = \sqrt{\left(j-m\right)\left(j+m+1\right)}, \tag{4.2.6}$$

and

$$C_{j,m-} = \sqrt{\left(j+m\right)\left(j-m+1\right)}, \tag{4.2.7}$$

respectively.

The equation 4.2.5 is a two-term difference-differential equation and the method of solving this kind of equation has been shown in Sect 10.3 of Ref [54] and is included in the Appendix A. We denote $\alpha_{j,m} = -\gamma\left(C_{j,m+}^2 + C_{j,m-}^2\right)$ and $\gamma_{j,m} = \gamma C_{j,m+}^2$. Then the solution of the reduced density matrix element $\rho_{j,m}$ at time t is

$$\begin{aligned}\rho_{j,m}(t) &= \exp\{\alpha_{j,m}t\}\,[\rho_{j,m}(0) \\ &\quad + \sum_{k=m+1} \frac{(1-\exp(-t))^{k-m}\,\gamma_{j,m}\gamma_{j,m+1}\cdots\gamma_{j,k-1}}{(k-m)!}\rho_{j,k}(0)].\end{aligned} \tag{4.2.8}$$

From equation 4.2.8, when the initial density matrix for the reduced density matrix is diagonalized, it is still diagonalized at time t. Because the spin-star system operator J_z is also diagonalized in the eigenspace $\{|\lambda, j, m\rangle\}$:

$$J_z = \sum_j n(j,N) \sum_{m=-j}^{m=j} m|\lambda,j,m\rangle\langle\lambda,j,m|, \tag{4.2.9}$$

the expectation value of the operator J_z is easily calculated as

$$\begin{aligned}\langle J_z(t)\rangle_S &= Tr_S\{J_z\rho_S(t)\} \\ &= \sum_j n(j,m) \sum_{m=-j}^{m=j} m\rho_{j,m}(t),\end{aligned} \tag{4.2.10}$$

where $\rho_{j,m}(t)$ is determined by the equation 4.2.8 and a given diagonalized initial density matrix $\rho_S(0)$.

The two-time correlation function of operator J_z is calculated by using quantum regression theorem [23] [54] [55] (see Appendix B)

$$\langle J_z(t+\tau)\,J_z(t)\rangle = Tr_S\left\{J_z\rho^{'}(\tau)\right\}, \tag{4.2.11}$$

where $\rho^{'}(0) = J_z\rho(t)$

The diagonal elements of $\rho^{'}(0)$ is

$$\rho^{'}_{j,m}\left(0\right) = m\rho_{j,m}\left(t\right), \tag{4.2.12}$$

and the diagonal elements of $\rho^{'}\left(\tau\right)$ is

$$\begin{aligned}\rho^{'}_{j,m}\left(\tau\right) &= \exp\left\{\alpha_{j,m}t\right\}[\rho^{'}_{j,m}\left(0\right) + \sum_{k=m+1}\frac{\left(1-\exp\left(-t\right)\right)^{k-m}\gamma_{j,m}\gamma_{j,m+1}\cdots\gamma_{j,k-1}}{(k-m)!}\rho^{'}_{j,k}\left(0\right)] \\ &= \exp\left\{\alpha_{j,m}\tau\right\}[m\rho_{j,m}\left(t\right) + \sum_{k=m+1}\frac{\left(1-\exp\left(-\tau\right)\right)^{k-m}\gamma_{j,m}\gamma_{j,m+1}\cdots\gamma_{j,k-1}}{(k-m)!}m\rho_{j,k}\left(t\right)].\end{aligned} \tag{4.2.13}$$

Therefore, the two-time correlation function of operator J_z is

$$\langle J_z\left(t+\tau\right)J_z\left(t\right)\rangle = \sum_{j} n\left(j,N\right)\sum_{m=-j}^{j} m\rho^{'}_{j,m}\left(\tau\right), \tag{4.2.14}$$

where $\rho^{'}_{j,m}\left(\tau\right)$ is obtained by substituting 4.2.8 into 4.2.13.

4.3 Gaussian approximation

With the help of two-time environment correlation function, the Gaussian approximation of the decoherence factor is (see Chapter 2)

$$f_{Gaussian}\left(t\right) = \exp\left(-2\int_0^t dt^{'}\int_0^{t^{'}} dt^{''}\langle J_z\left(t^{'}\right)J_z\left(t^{''}\right)\rangle\right), \tag{4.3.1}$$

where $\langle J_z\left(t^{'}\right)J_z\left(t^{''}\right)\rangle$ is the two-time correlation function 4.2.14.

Chapter 5

Conclusion

This thesis consists of two main parts. In Chapter 3 we have studied an exactly solvable spin-star model. Firstly, exact solutions of the reduced density matrix for the central spin has been plotted with various values for coupling strength λ, the initial bath temperature T, and the number of spins in the spin bath N. It has been shown that the coupling strength λ determines the full recurrence period, while the number of spins N increase the speed of fast oscillations in a full recurrence period. As a result, we have shown that the spin bath in our spin-star model is a non-Markovian and non-Gaussian environment. Secondly, we have applied several open quantum system methods on the spin-star model. The Born-Markov approximation is shown to be not applicable to our model even with a weak coupling strength, which is due to the time-independent bath correlation function. Finally, the comparison of NZ2 and TCL2 with the exact solutions for different regime suggests that the performances of Nakajima-Zwanzig and time-convolutionless methods depends on the form of the exact solution.

In Chapter 4 we have studied an open spin-star model. The open spin-star model in this thesis is not exactly solvable. The spin bath and the heat reservoir together can be approximated as a Gaussian environment when the central spin is only weakly coupled to the spin bath. The two-time correlation function of this Gaussian environment is obtained by using quantum regression theorem. We finally obtained a Gaussian approximation solution for the reduced dynamics of the central spin in the open spin-star model. More discussions about this approximation result are expected in the future work.

APPENDICES

A. Solution of Two-Term Difference-Differential Equation

In this appendix, we solve the equation

$$\dot{C}_m = \alpha C_m + \gamma_m C_{m+1} \quad m = 0, 1, \ldots, N, \tag{5.0.2}$$

assuming that $C_{N+1} = 0$.

Taking the Laplace transform of 5.0.2, we have

$$\tilde{C}_m = \frac{1}{z - \alpha_m} \left[C_m(0) + \gamma_m \tilde{C}_{m+1} \right]. \tag{5.0.3}$$

Set $m = N$ in this and use the given condition $\tilde{C}_{N+1} = 0$ to obtain

$$\tilde{C}_N = \frac{1}{z - \alpha_N} C_N(0). \tag{5.0.4}$$

Set $m = N - 1$, $N - 2$, …, successively in 5.0.3 to get

$$\tilde{C}_m = \frac{1}{z - \alpha_m} \left[C_m(0) + \sum_{k=1}^{N-m} C_{m+k}(0) \prod_{l=1}^{k} \frac{1}{z - \alpha_{m+l}} \gamma_{m+l-1} \right]. \tag{5.0.5}$$

The inverse Laplace transform of 5.0.5 gives $C_m(t)$,

$$\begin{aligned} C_m(t) = {} & \exp\{\alpha_m t\} \left[C_m(0) \right. \\ & \left. + \sum_{k=m+1} \frac{(1 - \exp(-t))^{k-m} \gamma_m \gamma_{m+1} \cdots \gamma_{k-1}}{(k-m)!} C_k(0) \right] \end{aligned} \tag{5.0.6}$$

We can verify the correctness of this solution by substituting it in 5.0.2.

B. Quantum regression theorem

In this appendix, we consider the two-time correlation function of operators $\hat{A}^{(S)}$ and $\hat{B}^{(S)}$ of system S. By definition,

$$\langle \hat{A}^{(S)}\left(t+\tau\right)\hat{B}^{(S)}\left(\tau\right)\rangle = Tr_{R+S}\left\{\hat{A}^{(S)}\left(t+\tau\right)\hat{B}^{(S)}\left(t\right)\hat{\rho}\left(0\right)\right\}. \tag{5.0.7}$$

The operators are in the Heisenberg picture involved by the total Hamiltonian $\hat{H}$:

$$\hat{A}\left(t\right) = e^{i\hat{H}t/\hbar}\hat{A}e^{-i\hat{H}t/\hbar}. \tag{5.0.8}$$

By using equation 5.0.8 and the cyclic property of trace, the definition of the two-time correlation function 5.0.7 leads to

$$\begin{aligned}\langle \hat{A}^{(S)}\left(t+\tau\right)\hat{B}^{(S)}\left(t\right)\rangle &= Tr_{R+S}\left\{\hat{A}^{(S)}\left(\tau\right)\hat{B}^{(S)}\exp\left(-\frac{i}{\hbar}\hat{H}t\right)\hat{\rho}\left(0\right)\exp\left(\frac{i}{\hbar}\hat{H}t\right)\right\}\\ &= Tr_{R+S}\left\{\hat{A}^{(S)}\exp\left(-\frac{i}{\hbar}\hat{H}\tau\right)\hat{B}^{(S)}\hat{\rho}\left(t\right)\exp\left(\frac{i}{\hbar}\hat{H}\tau\right)\right\}\\ &= Tr_{R+S}\left\{\hat{A}^{(S)}\exp\left(\hat{\hat{L}}\tau\right)\left(\hat{B}^{(S)}\hat{\rho}\left(t\right)\right)\right\}\\ &= Tr_{S}\left\{\hat{A}^{(S)}Tr_{R}\left\{\exp\left(\hat{\hat{L}}\tau\right)\left(\hat{\rho}^{'}\left(0\right)\right)\right\}\right\},\end{aligned} \tag{5.0.9}$$

where $\hat{\rho}^{'}\left(0\right) = \hat{B}^{(S)}\hat{\rho}\left(t\right)$.

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