Aspects of Decoherence in Qubit Systems

by

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Abstract

We present a theoretical discussion of various aspects of the dynamics of information in quantum systems of qubits. We begin by reviewing ideas about entanglement and information in systems of qubits, different models for realistic qubits coupled to an external environment, how this causes the loss of information stored in qubits, and some practical designs for qubits that have been created. Then we study how the state of many-body systems can be decomposed in terms of its different subsystems and derived a hierarchy of equations describing the motion of these different parts. We show that in a qubit system, the central objects in this hierarchy are correlators between different components of different qubits. Systems where the environment coupled to a central qubit is a “spin bath” of environmental qubits are then considered in detail and we find that information lost by the central qubit is transferred via a cascade to higher and higher order correlations with the environment. We discusses this process in the realistic example of an “Fe$_8$” magnetic molecule qubit. Finally we discuss simple models of the dynamics of many entangled qubits.
Lay Summary

A quantum computer will be able to solve problems much faster than a traditional computer. Quantum computers rely on the quantum behaviour of matter, typically seen at the atomic scale. So far only small quantum computers, consisting of a few dozen quantum bits or “qubits”, have been built and tested. Information is stored and used in a quantum computer when qubits have correlations between themselves and within the qubit. The main obstacle to development of a large quantum computer is that information leaks out of the system when the qubits build correlations with the environment. We have studied a number of different theoretical models of realistic systems consisting of various multiple qubits arrangements (and their environment). For these models we have worked out the exact nature of the spurious correlations that arise with the environment, and have thereby developed a picture of how these systems lose information to the environment.
Preface

Figure 3.8 is reproduced from [40] with permission, figure 6.2 was provided by Philip C. E. Stamp. The rest of the material in this thesis is the original work of the author, Timothy Cox. All work was supervised by Philip C. E. Stamp including guidance in analyses and project direction. Chapters 2-4 and appendices A-C of this thesis are adapted from a draft of an original manuscript published in a peer-reviewed journal with Timothy Cox as the primary author [18]. All other chapters are original work, first published in this document.
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6.8 The $n$–partite correlation strength for the degeneracy blocking model described in section 6.1.2. and the definition for $c_n$ (6.40). In the case plotted there are $N = 100$ bath spins, their couplings are all $\omega_0 = \frac{1}{2}\Delta_0$ (so $\frac{1}{2}\sqrt{N}\omega_0 = \Delta_0$), and the initial reduced density matrix for the system is $\bar{\rho}_S(0) = \frac{1}{2}(1 + \tau^x)$.

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8.1 Structure of the Fe$_8$ molecule. The crosshatched circles are the Fe$^{3+}$ ions, the hatched circles are the oxygen atoms, and the empty circles represent, in order of decreasing size, nitrogen and carbon atoms. [Reprinted figure with permission, from D Gatteschi, A. Caneschi, L., R. Sessoli, Science, 265, 1054 (1994), 40. Copyright 1994 by the American Association for the Advancement of Science.]
8.2 The energy of the electronic spin vector in the Fe$_8$ molecule. Both the main plot and the inset plot shaded colour shows the semiclassical energy of the electronic spin in the Fe$_8$ molecule as a function of its direction on the Bloch sphere, when the applied field is $\mu_0 H_\perp = 2.5$ T $\hat{y}$. The scale shown on the right gives the energy/$k_B$ in Kelvins. The black bullets (●) mark the positions of the energy minima where the qubit states are localised. The dotted black line marks the semiclassical tunneling route. The inset plot is the same as the main plot but viewed from a different angle.

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8.8 A plot of correlators between the bath spins and the central spin, for the case of a single Fe$_8$ molecule coupled to its $^1$H nuclear spin bath, when we have averaged over the different choices for sites $i$ and $j$. The dotted blue curve is $\langle \tau^z \sigma^x_i \sigma^x_j \rangle = \langle \tau^z \sigma^y_i \sigma^y_j \rangle$ and the dashed green curve is $\langle \tau^y \sigma^z_i \sigma^z_j \rangle$.

8.9 The initial stages of decoherence in an Fe$_8$ qubit, when we have averaged over the different choices for bath spins $i$ and $j$. The top figure shows components of the central qubit $\langle \tau \rangle$, the solid red curve is $\langle \tau^x \rangle$, the dashed green curve is $\langle \tau^y \rangle$, and the dotted blue curve is $\langle \tau^z \rangle$. The bottom figure is plot of correlators between the pairs of bath spins and the central spin, the dotted blue curve is $\langle \tau^z \sigma^x_i \sigma^x_j \rangle = \langle \tau^z \sigma^y_i \sigma^y_j \rangle$ and the dashed green curve is $\langle \tau^y \sigma^z_i \sigma^z_j \rangle$.

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Chapter 1

Introduction

This thesis concerns the dynamics and stability of information contained in qubits, a quantum analog of the classical bit, which stores information in computers [78]. There is a large effort underway in the design and construction of quantum computers containing a large number of qubits. Such a computer would be able to solve complicated problems significantly faster than a classical computer [34]. The main difficulty in constructing a quantum computer is that quantum information is fragile, it is lost as qubits become entangled with the outside world (the environment) [24, 25].

The key questions addressed in this thesis are: How can we divide the information stored in a many qubit system? How does is that information lost into the environment? Where does the information go when it lost? And how does the rate of information lost depend on the size of our system.

Before we turn to these questions, we need to discuss some more background material, which is presented in the remainder of this chapter. First the density matrix description of the quantum state, qubits, quantum entanglement, and how one can use quantum mechanics speed up computations is briefly discussed. In particular we discuss the link between “information”, entanglement and correlators of qubit components. In section 1.6 previous models for the coupling of a “central system” of qubits to an environment are discussed. In section 1.8 two different qubit designs are reviewed, paying particular attention to their coupling to the environment which we hope to model. Following that we outline the remaining content of the thesis.

1.1 The Quantum State

In quantum mechanics the notion of a “state” is richer than that in classical mechanics. This is because of the superposition principle, which means that any linear combination of basis states can define a state. Consider a prototypical example of a \( d \)-level quantum system, a single particle which may hop between \( d \) “sites” labeled \( j = 1, 2, \ldots, d \). Classically, to specify the state of the particle one would simply have to give its position (one integer). While quantum mechanically, the wave function \( |\psi\rangle \) which defines the state of the particle, can in general be in any superposition in
the \( d \)-dimensional Hilbert space\[91\]

\[
|\psi\rangle = \sum_{j=1}^{d} c_j |j\rangle,
\]
(1.1)

with the restriction that \( \sum_{j=1}^{d} |c_j|^2 = 1 \), and states related by an arbitrary phase rotation are identical. So in the quantum case one needs to specify \( d \) complex numbers \( \{c_j\} \) with one constraint. So one needs \( 2d - 2 \) real numbers to fully describe the state.

The extra information contained in a quantum state and the fact that it can be all manipulated “in parallel” is the basis for the operation of a quantum computer \[21\]. Currently there is a large amount of research being done to produce such a computer, which would be able to solve problems which would be intractable on a traditional “classical” computer.

The wave function such as (1.1) describes a pure state of a completely isolated system. If we are studying a system which can be entangled with an external “environment” (this is strictly true for all experimental systems), then the state of the system \( \mathcal{S} \) is defined by its reduced density matrix \( \bar{\rho}_S \). The reduced density matrix \( \bar{\rho}_S \) can be any operator on the Hilbert space that satisfies the axioms \[91\]:

1. The density matrix has trace one, \( \text{tr}\bar{\rho}_S = 1 \).

2. The density matrix is Hermitian, \( \bar{\rho}_S^\dagger = \bar{\rho}_S \).

3. The density matrix is positive semi definite, all its eigenvalues \( \lambda_n \geq 0 \).

Specifying a \( d \times d \) Hermitian matrix requires specifying \( d^2 \) real numbers, so that in general the reduced density matrix of a system can be specified by \( d^2 - 1 \) real numbers as its trace is fixed to one. Of course some possible choices for these \( d \) real numbers will be invalid, they will result in a density matrix which has negative eigenvalues. So there is a region of this \( d^2 - 1 \) dimensional space which give valid density operators. We see that the quantum state is much more complicated than a classical state. We can construct a set of observables which this extra information specifies. If we define the sets of Hermitian operators,

\[
\hat{P}_j \equiv |j\rangle\langle j| \quad (1.2)
\]

\[
\hat{r}_{jk} \equiv |j\rangle\langle k| + |k\rangle\langle j| \quad (j \neq k) \quad (1.3)
\]

\[
\hat{c}_{jk} \equiv -i |j\rangle\langle k| + i |k\rangle\langle j| \quad (j \neq k). \quad (1.4)
\]

Together these form a basis for the real Hilbert space of possible \( d \times d \) Hermitian matrices and then the density matrix takes can be written in terms of these operators,

\[
\bar{\rho}_S = \sum_{j=1}^{d} \langle \hat{P}_j \rangle \hat{P}_j + \frac{1}{2} \sum_{j=1}^{d} \sum_{k=1}^{j-1} \langle \hat{r}_{jk} \rangle \hat{r}_{jk} + \frac{1}{2} \sum_{j=2}^{d} \sum_{k=1}^{j-1} \langle \hat{c}_{jk} \rangle \hat{c}_{jk}. \quad (1.5)
\]
In the expression (1.5) the density matrix is written in terms of expectations of a complete set of \( d^2 \) observables \( \{ \hat{P}_j, \hat{r}_{jk}, \hat{s}_{jk} \} \), where only \( d^2 - 1 \) are independent due to the trace condition \( \sum_{k=1}^{d} \langle P_k \rangle = 1 \). If we allowed our classical system to be described by a probability distribution with one probably for each site, we would only require \( d - 1 \) real values to specify this probability distribution. This is equivalent to specifying the values of the diagonal values of the density matrix \( \{ \langle P \rangle \} \) only and gives us an interpretation to these values. The values of expectations of the off diagonal operators \( \hat{c}_{jk} \) and \( \hat{r}_{jk} \) are intrinsically quantum and are present when the system is in a coherent superpositions of the different states. A picture of the classical limit is that there is some “natural basis” in which coupling to an environment means that these off diagonal expectations die down rapidly with time. This process is called decoherence.

### 1.2 Qubits

Most practical implementations of a quantum computer will store and operate on quantum information stored in the quantum states of qubits. Qubits are the quantum analogs of classical bits. Classical bits are hypothetical systems that may be in one of two states which we will refer to as -1 and 1 (this is slightly different than the traditional convention quantum information convention of 0 and 1 but it will make the notation we use in the study of the dynamics simpler). Qubits or quantum two level systems on the other hand are in general described by a density matrix

\[
\rho = \begin{pmatrix}
\langle 1|\rho|1 \rangle & \langle 1|\rho| -1 \rangle \\
\langle -1|\rho|1 \rangle & \langle -1|\rho| -1 \rangle
\end{pmatrix}
\]  

(1.6)

whose diagonal elements give the probability of finding the qubit in either of the states and whose off diagonal elements describe coherent quantum superposition of these states.

There are a variety of designs for creating qubits for use in quantum information. All practical qubits will be the result of arranging a complicated system in such a way that only two states are accessible to the system. One way to achieve this is to take a system which naturally has two levels such as an electronic or nuclear spin and isolate it from the environment, for example spins of magnetically trapped ions [15] or electronic spins in defect in a semiconductor [54]. In such a system the two qubit states are the state where the spin is up \( |1\rangle = |\uparrow\rangle \) and down \( |-1\rangle = |\downarrow\rangle \) with respect to the quantisation axis. Sometimes in this thesis we will use the spin-\( \frac{1}{2} \) language to refer to qubits which are not necessarily half spins, referring to \( |-1\rangle \) as “spin down” and \( |1\rangle \) as “spin up”. Another approach is to isolate two low lying energy levels of a system so that exciting the system at a specific frequency only causes transitions between these levels. Examples of qubit designs utilising this approach include the various different qubit designs based on superconducting circuits [64] and magnetic molecules [100], which we discuss in more detail in section 1.8.
For a single qubit we can build a basis of all possible operators which operate the two dimensional qubit Hilbert space of states using the Pauli matrices and the identity,

\[ \sigma^x = |1\rangle\langle-1| + |-1\rangle\langle1| = \hat{r}_{1-1} \]
\[ \sigma^y = i|1\rangle\langle-1| - i|-1\rangle\langle1| = \hat{c}_{1-1} \]
\[ \sigma^z = |1\rangle\langle1| - |-1\rangle\langle-1| = \hat{P}_1 - \hat{P}_{-1} \]
\[ I = |1\rangle\langle1| + |-1\rangle\langle-1| = \hat{P}_1 + \hat{P}_{-1}. \]

The single qubit density matrix can be conveniently represented in terms of this basis [31, 32, 78, 82]

\[ \rho = \frac{1}{2}(1 + \langle \sigma \rangle \cdot \sigma). \]

This representation is discussed in more detail and generalised to systems with multiple qubits in chapter [3]. The various terms in the above representation for the density matrix have the following interpretations when the z direction is our quantisation axis: The \( \langle \sigma_z \rangle \) information tells us about classical probabilities of being in states \(|\pm 1\rangle\) which are \( p_{\pm} = \frac{1}{2}(1 \pm \langle \sigma_z \rangle) \) and the off-diagonal correlators \( \langle \sigma_x \rangle, \langle \sigma_y \rangle \) tell us about quantum coherent quantum superposition which are intrinsically non-classical.

We can also write any possible effective Hamiltonian which govern the dynamics of a single qubit system in terms of the Pauli operators. Suppose the energy of the state \(|\pm 1\rangle\) is \( \epsilon_{\pm} \) then the diagonal part of the effective Hamiltonian is

\[ H_d = \epsilon_+ |1\rangle\langle1| + \epsilon_- |-1\rangle\langle-1| = \frac{\epsilon_+ + \epsilon_-}{2} + \left( \frac{\epsilon_+ - \epsilon_-}{2} \right) \sigma^z. \]

If we allow tunneling between the two states with an amplitude of \( \Delta_0/2 \) accompanied by a phase shift of \( \phi \) (this is the most general tunneling element), then the tunneling Hamiltonian is,

\[ H_t = \frac{1}{2} \left( \Delta_0 e^{i\phi} |1\rangle\langle1| + \Delta_0 e^{-i\phi} |-1\rangle\langle-1| \right) = \frac{\Delta_0}{2} (\cos \phi \sigma^x + \sin \phi \sigma^y). \]

The total effective Hamiltonian is then \( H = H_d + H_t \). We see that in the absence of an energy splitting the ground state of the qubit system is a superposition of \(|1\rangle\) and \(|-1\rangle\).

The qubit levels could be either two levels of a “natural” two level system (e.g. the spin of spin-\( \frac{1}{2} \) particle) or two low lying energy levels a more complicated system. One important example this second type of qubit, which we will call an effective qubit, is a continuous system where the co-ordinate \( Q \) has a double well type potential like that shown in figure [1.1]. To see how this pans out in practice we have to consider an actual system, we will do this in section [1.8].
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Figure 1.1: The potential energy for an idealised effective qubit as a function of $Q$. There are two minima at $Q_{\pm}$. If we assume the two potential wells are deep, we can expand the potential around these minima and find an approximate lowest energy states with energies $\epsilon_{\pm}$ in each of the minima, these states act as our qubit states.

1.3 Entanglement

There is another intrinsically quantum phenomena that can occur when we have more than one quantum systems interacting, entanglement. Here we only give a rudimentary introduction and give a short explanation of what entanglement is, how it is used in quantum computing, and how it can be quantified and measured. Entanglement in qubit systems is discussed in more details in chapter 3.

Quantum entanglement occurs when systems made up of multiple parts (for example particles) are in a superposition of states, for which each of the parts of the system is different. For example consider two qubits in the state

$$|\psi_e\rangle = \frac{1}{\sqrt{2}}|+1\rangle + \frac{1}{\sqrt{2}}|1-1\rangle,$$

where is a superposition of two states for which both the qubits are different. This means the properties of qubit one and two are intrinsically linked. It has been shown that this kind of entanglement is vital for the fast operation of a quantum computer [53]. The density matrix representing the entangled state with wave function, $|\psi_e\rangle$ in equation (1.15) is,

$$\rho_{12} = \frac{1}{2}(|11\rangle\langle 11| + |1-1\rangle\langle -1-1| + |11\rangle\langle -1-1| + |1-1\rangle\langle 11|).$$
From equation (1.16) which we see that the entangled qubits “share” off diagonal elements in the density matrix. Suppose we traced the second qubit out, then the reduced density matrix, which encodes the information stored in the first qubit alone is,

\[ \bar{\rho}_1 = \frac{1}{2} (|1\rangle\langle1| + |−1\rangle\langle−1|) = \frac{1}{2} I. \]  

(1.17)

The reduced state of the first qubit is completely described by a classical probability distribution, with the $|±1\rangle$ states having equal probability. So the expectation of any component of the first qubit’s polarisation $⟨σ_1⟩$ is zero. The same applies to the second qubit. However if both qubits are measured, one will find that they are always aligned with one another along the $z$ axis and a measurement of one of the qubits with respect to this axis, will completely predict the outcome of the measurement of the other. In this way the two spins are entangled. These kind of states, particularly in the case where the two qubits are spins that are spatially separated, were at the heart of early controversies about quantum mechanics [30].

We will review some of the formal theory of quantifying entanglement in the next section in more detail. But for now we consider the qualitative features of an arbitrary many qubit quantum state consisting of $N$, qubits. Define $s = (s_1, s_2, \ldots, s_N)$, where $s_i = ±1$, an arbitrary $N$ qubit states wave function can be written

\[ |Ψ_N⟩ = \sum_\mathcal{Z} a_\mathcal{Z}|\mathcal{Z}\rangle. \]  

(1.18)

Where there are $4^N − 1$ free real parameters (the $−1$ accounts for the fact the wave function must be normalised) in the coefficients $\{a_\mathcal{Z}\}$. It is clear that all states for which more than one of the $\{a_\mathcal{Z}\}$ coefficients are non-zero have entanglement, and moreover states where more than two of these coefficients are non-zero have entanglement involving at least three qubits. Continuing this line of argument, one can see that generic $N$ qubit states are highly entangled. So that much of information contained in the wave functions specifies these entanglements. In the next section we discuss ways to quantify and measure this entanglement.

1.4 Quantifying and Detecting Quantum Entanglement

It is desirable to quantify the “amount” of entanglement in different states. In a system consisting of multiple subsystems there are in general many different types of entanglement possible. There is a large amount of literature on quantifying entanglement, see the reviews [3, 43, 47, 113] for an introduction. Here we discuss some of the simpler formal definitions of entanglement, measures of entanglement, and touch on some of the complexity of the problem in the multipartite case.
1.4.1 Bipartite Entanglement

We start by considering a pure state, of a system which consists of two subsystems $A$ and $B$. Subsystems $A$ and $B$ are said to be entangled if the total density matrix $\rho_{AB}$ cannot be written as a product state \[47\]. That is, no state vectors $|\psi_A\rangle$ and $|\psi_B\rangle$ in the Hilbert spaces for the subsystems exist such that

$$\rho_{AB} = |\psi_A\rangle\langle\psi_A||\psi_B\rangle\langle\psi_B|.$$ \hspace{1cm} (1.19)

A natural measure of how entangled the subsystem $A$ is with the subsystem $B$ is the von Neumann entropy $S(\rho_{AB})$ defined by,

$$S(\rho_{AB}) = -\text{tr}\bar{\rho}_A \log \bar{\rho}_A = -\text{tr}\bar{\rho}_B \log \bar{\rho}_B.$$ \hspace{1cm} (1.20)

Where $\bar{\rho}_A$ and $\bar{\rho}_B$ are the reduced density matrices on $A$ and $B$ respectively, defined by tracing out the complementary set,

$$\bar{\rho}_A = \text{tr}_B \rho_{AB}$$ \hspace{1cm} (1.21)

$$\bar{\rho}_B = \text{tr}_A \rho_{AB}.$$ \hspace{1cm} (1.22)

It can be shown that von Neumann entropy can be interpreted in terms of the information contained in the reduced density matrix. The von Neumann of a pure quantum state is equal to the number qubits necessary to transmit the quantum information contained in the reduced density matrix $\bar{\rho}_A$ (or equivalently $\bar{\rho}_B$) \[93\]. When $A$ and $B$ are fully entangled $\bar{\rho}_A$ contains no information and $S(\rho_{AB}) = 0$. This is the case for the qubit example in section [1.3].

Note that, while the von Neumann entropy has a nice information theoretic interpretation, there are many other quantities\[111\] which behave monotonically under local transformations and can be used to characterise entanglement. Such quantities are called entanglement monotones. One such monotone, which is in general easier to calculate than the von Neumann entropy, is the linear entropy $S_L(\rho_{AB})$,

$$S_L(\rho_{AB}) = 1 - \text{tr}\bar{\rho}_A^2.$$ \hspace{1cm} (1.23)

When the linear entropy is zero, the reduced density matrices $\bar{\rho}_A$ and $\bar{\rho}_B$ represent pure states and the sub systems are not entangled. We note for future reference that the quantity $\text{tr}(\bar{\rho}_A^2)$, which is one when $\bar{\rho}_A$ represents a pure state and less than one otherwise, is called the purity of $\bar{\rho}_A$.

Now consider the case where $\bar{\rho}_{AB}$ represents a mixed state of the bipartite system $AB$. We say that a density matrix represents a genuinely entangled, state if it cannot be written as an ensemble average of $N_s$ separable states $|\psi^i_A\rangle|\psi^i_B\rangle$ ($i = 1, \ldots, N_s$), with probabilities $\{p_i\}$. That is if $\bar{\rho}_{AB}$ cannot be written,

$$\bar{\rho}_{AB} = \sum_{i=1}^{N_s} p_i |\psi^i_A\rangle\langle\psi^i_A||\psi^i_B\rangle\langle\psi^i_B|,$$ \hspace{1cm} (1.24)
for any ensemble \( \{ p_i, |\psi_i^A\rangle|\psi_i^B\rangle\} \), then the subsystems \( A \) and \( B \) are genuinely entangled. This definition of entanglement distinguishes between, states which are ensembles of classical states in which \( A \) and \( B \) are correlated and states which have genuine quantum entanglement. The appropriate generalisation of the von Neumann entropy to mixed states is the entropy of formation \( S_F(\bar{\rho}_A) \),

\[
S_F(\bar{\rho}_A) = \inf_{\{ p_i, |\psi_i^A\rangle|\psi_i^B\rangle\}} \sum_i p_i S(|\psi_i^A\rangle\langle\psi_i^A||\psi_i^B\rangle\langle\psi_i^B|).
\]

(1.25)

Here \( \inf_{\{ p_i, |\psi_i^A\rangle|\psi_i^B\rangle\}} \) denotes the infimum (or equivalently the greatest lower bound) over all possible decompositions of the density matrix which are of the form (1.24). This makes the entropy of formation difficult to calculate in general. There are some cases where simpler formulae may be used to calculate the entanglement of formation, one such case is where \( \mathcal{A} \) and \( \mathcal{B} \) both consist of single qubits [119]. The entanglement of formation has the same interpretation in terms of information as the von Neumann entropy does for pure states.

**Detecting Bipartite Entanglement**

Entanglement can be detected by measuring quantities called *entanglement witnesses*. For example consider a system consisting of two qubits \( \sigma_1 \) and \( \sigma_2 \). The operator \( \hat{W}(\hat{a}, \hat{a}', \hat{b}, \hat{b}') \) defined by [104],

\[
\hat{W}(\hat{a}, \hat{a}', \hat{b}, \hat{b}') \equiv \frac{1}{4} \left[ 2I - (\hat{a} \cdot \sigma_1)(\hat{b} \cdot \sigma_2) - (\hat{a} \cdot \sigma_1)(\hat{b}' \cdot \sigma_2) + (\hat{a}' \cdot \sigma_1)(\hat{b} \cdot \sigma_2) - (\hat{a}' \cdot \sigma_1)(\hat{b}' \cdot \sigma_2) \right],
\]

(1.26)

for a given set of unit vectors \( \hat{a}, \hat{a}', \hat{b}, \) and \( \hat{b}' \). Measuring a value of \( \langle \hat{W}(\hat{a}, \hat{a}', \hat{b}, \hat{b}') \rangle < 0 \) indicates a violation of the Bell inequalities [6], in the form derived by Clauser et. al. [16]. So \( \hat{W}(\hat{a}, \hat{a}', \hat{b}, \hat{b}') \) is an entanglement witness as \( \langle \hat{W}(\hat{a}, \hat{a}', \hat{b}, \hat{b}') \rangle < 0 \) indicates the two qubits are entangled. Note that \( \langle \hat{W}(\hat{a}, \hat{a}', \hat{b}, \hat{b}') \rangle < 0 \) for a given set of \( \hat{a}, \hat{a}', \hat{b}, \) and \( \hat{b}' \) is a sufficient condition for entanglement, but not a necessary condition. For example with the parameters [78] \( \hat{a} = \hat{z}, \hat{b} = -\left( \frac{\hat{x} + \hat{z}}{2} \right), \hat{a}' = \hat{x}, \hat{b}' = \frac{\hat{z} - \hat{x}}{2} \), for the entangled state \( |\psi\rangle = \frac{1}{\sqrt{2}}(|11\rangle + |1 - 1\rangle) \) one finds,

\[
\langle \hat{W} \left( \hat{z}, \hat{x}, -\left( \frac{\hat{x} + \hat{z}}{2} \right), \frac{\hat{z} - \hat{x}}{2} \right) \rangle = \frac{1}{2} \left( 1 + \sqrt{2} \right) > 0.
\]

(1.27)

So the witness \( \hat{W} \left( \hat{z}, \hat{x}, -\left( \frac{\hat{x} + \hat{z}}{2} \right), \frac{\hat{z} - \hat{x}}{2} \right) \) fails to detect the entanglement in \( |\psi\rangle \). In general different witnesses may detect different “types” of entanglement. As entanglement witnesses are always represented by Hermitian operators in a multi-qubit system any witness can be constructed from correlators of different spin components.
1.4.2 Multipartite Entanglement

Now consider a multipartite system $\mathcal{S}$, composed of $N$ subsystems $\{i\}$, $i = 1, \ldots, N$. Suppose the (in general mixed) state of $\mathcal{S}$ is represented by the density matrix $\tilde{\rho}_S$, then the state is said to be fully separable and therefore not genuinely entangled if it can be written [27],

$$\tilde{\rho}_S = \sum_{a=1}^{N_s} p_a \prod_{i \in S} \tilde{\rho}_a^i. \quad (1.28)$$

That is, if $\tilde{\rho}_S$ represents a genuinely entangled state, it cannot be written as an ensemble average over a number, $N_s$, of states, $\tilde{\rho}_S^a = \prod_{i \in S} \tilde{\rho}_a^i$ ($a = 1, \ldots, N_s$), which are a product of local density matrices.

A fully separable state contains no entanglement between any of its subsystems. A state can fail to be fully separable in a large number of ways. For instance, a state of a system containing a large number of subsystems, can fail to be fully separable if just two of its subsystems (say subsystems “1” and “2”) are entangled. Such a state would be partially separable, in the sense that its density matrix could be written $\sum_{a=1}^{N_s} p_a \tilde{\rho}_a^{12} \prod_{i \in S \setminus \{1, 2\}} \tilde{\rho}_a^i$. In general we can ask about the separability of a state of the system $\mathcal{S}$ with respect to any partition of $\mathcal{S}$ into number of disjoint subsystems $\{A_\ell\}$. A density matrix $\tilde{\rho}_S$ is separable with respect to the partition $\{A_\ell\}$ if it can be written as an ensemble average of product states over that partition [27],

$$\tilde{\rho}_S = \sum_{a=1}^{N_s} p_a \prod_{\ell} \tilde{\rho}_a^A_\ell. \quad (1.29)$$

The number $B_N$ of partitions containing $N$ “elementary subsystems” into which $\mathcal{S}$, can be divided is called the Bell number and is well studied in the field of combinatorics [36]. The Bell number grows super exponentially with the $N$ [36]. So we see, that even just considering the separability of a many party density matrix, characterising the entanglement of a multipartite system can be very complicated. A large number of entanglement witnesses have been derived to characterise different types of multipartite entanglement, see [43] for a review. In this thesis we will avoid most of the complications of characterising the many different types of multipartite entanglement, by focusing on the study of the dynamics of the correlation functions, which can be used to construct any entanglement witnesses.

1.5 Quantum Computing

Quantum algorithms have been designed, which would be able to solve many large problems much faster than traditional classical algorithms [78]. These algorithms would have to be run on a quantum computer. Quantum computing has the potential to revolutionist the field of computation allowing the fast solutions to problems,
which would be unsolvable with a classical computer.

We saw in section 1.3, that most of the information in many qubit systems, is stored in the entanglements between the various qubits. There is good reason to believe that the information stored in the entanglements is vital for quantum computing. This because of quantum parallelism, the ability for a quantum computer to be able perform a set of operations on a state which is the superposition of multiple input states and produce the desired output for all the inputs at once (i.e. repeat the calculation multiple times in parallel).

In most designs for a quantum computer the information is stored and the calculations are performed using a set of qubits. This type of computer would consist of a set of qubits, an apparatus that could manipulate these qubits, and perform projective measurements on the qubits. DiVincenzo described a list of requirements for the operation of such a computer. The relevant criteria for the work in this thesis are that the information stored on the set of qubits survives long enough so that the computation can take place.

In later chapters of this thesis we will consider the dynamics systems consisting multiple qubits, and try and understand how they loss their information to the environment. In order to prepare for this work, in the next section we will discuss previous models for qubits coupled to an environment.

1.6 Models of the Quantum Environment

Here we review several models commonly used to describe the dynamics of a “central” quantum system coupled to an “environment”. As with the rest of this thesis we are interested in how the central system losses information to the environment and the problem of decoherence. In particular we consider the case where the central system consists of a set of qubits.

We will discuss two models where the full quantum dynamics of the environment are modeled as a “bath” containing a large number of environmental modes. We consider the cases where the environment consists of a bath of oscillator modes in section 1.7.1 and a bath of qubit modes in section 1.7.2.

1.7 The Environment as a Quantum System

As the environment is a system in its own right, the most complete model of a central system coupled to an environment will treat both the system and the environment on an equal footing, using an effective Hamiltonian which couples the system modes and environment.
In general the low energy effective Hamiltonian describing the coupled system and environment, is obtained by “integrating out” dynamics which occur at higher energies. This results in a description of the system in terms of a number of effective variables, which are important at the energy scales in which the system is probed. For a central system of \( N_S \) qubits \( \{\tau_a\}, a \in \{1, 2, \ldots, N_S\} \), in many cases this procedure leads to models where the low energy dynamics of the environment is modeled by “baths” containing two different types of modes, (i) delocalised modes such phonons which may be represented as oscillators \([13, 65]\) and (ii) localised modes such as spin and charge defects which may be represented as qubits or spins \([83, 86, 109, 122]\). In this section we review some of the work that has been done on these models. First we discuss the oscillator bath and how it can be treated using the influence functional method developed by Feynman and Vernon \([33]\). Then we discuss the spin bath and its effect on both “emergent” two level systems and spin half systems.

### 1.7.1 Oscillator bath models

The Hamiltonian for a set of qubits coupled to a “bath” consisting of a large number, \( N_o \) of harmonic oscillators, with coordinates \( \{Q_i\} \), and momenta \( \{P_i\} \) (for \( i = 1, \ldots, N_p \)) is,

\[
H = \frac{1}{2} \sum_{a=1}^{N_S} h_a \cdot \tau_a + \frac{1}{2} \sum_{a=1}^{N_S} \sum_{b \neq a}^{N_S} u_{ab}^{\mu\nu} \tau_a^\mu \tau_b^\nu + \sum_{a=1}^{N_S} \sum_{i=1}^{N_o} \Lambda_a^{\mu} r_i^\mu Q_i^\mu + \sum_{i=1}^{N_o} \left( \frac{P_i^2}{2m_i} + \frac{m_i \omega_i^2 Q_i^2}{2} \right).
\]

The oscillators are coupled to the central qubits with the constants \( \Lambda_a^{\mu} \), the \( i \)'th oscillator has natural frequency \( \omega_i \) (in the absence of the influence from qubits), mass \( m_i \) and we have allowed the central qubits to have a pairwise coupling \( u_{ab}^{\mu\nu} \).

The problem of a single qubit coupled to an oscillator bath has been studied extensively \([13, 65, 114]\), using the influence function method originally developed by Feynman and Vernon \([33]\), which is described below. More general environments for example a spin bath may be mapped to the problem of a bath of oscillators coupled to a central spin \([86]\), however such mappings are generally only valid when the coupling to the environmental modes are weak \([86]\). If the oscillators are modes of a delocalised field (eg the phonon field in a crystal hosting the qubit) this kind of coupling weak emerges naturally.

**Influence Functional**

The influence functional method is based on the path integral expression for the density matrix \( \rho(q, Q; q', Q'; t) \), as a function of the general system co-ordinates \( q, q' \) and bath co-ordinates \( Q, Q' \). At time \( t \) the density matrix is related to the
initial density matrix by [33],
\[
\rho(q, Q; q', Q'; t) = \int d\tilde{Q} \int d\tilde{Q}' \int d\tilde{q} \int d\tilde{q}' U(q, Q, t; \tilde{q}, \tilde{Q}, 0) \rho(\tilde{q}, \tilde{Q}; q', Q'; 0) U^*(q', Q', t; \tilde{q}', \tilde{Q}', 0).
\] (1.31)

\(U(q, Q, t; \tilde{q}, \tilde{Q}, 0)\) is a propagator matrix element, which has the following path integral representation. Each path accumulates a phase according to the action \(S[q, Q]\) of that path, then these paths are summed over in a path integral,
\[
U(q, Q, t; \tilde{q}, \tilde{Q}, 0) = \int_{x(0)=q}^{x(t)=Q} \mathcal{D}x \int_{x'(0)=q'}^{x'(t)=Q'} \mathcal{D}x' e^{-i\frac{\pi}{\hbar} \left[ S_0[x] - S_0[x'] \right]} \rho_S(\tilde{q}, \tilde{Q})F[x, x'].
\] (1.32)

Assuming that the initial density matrix is separable, so that
\[
\rho(q, Q; q', Q'; 0) = \bar{\rho}_S(q; q'; 0) \bar{\rho}_B(Q; Q'; 0)
\] (1.33)

and that the action separates \(S[q, Q] = S_0[q] + S_B[q, Q]\), then one has the following expression for the reduced density matrix of the system,
\[
\bar{\rho}_S(q, q'; t) = \int d\tilde{q} \int d\tilde{q}' \int_{x(0)=q}^{x(t)=Q} \mathcal{D}x \int_{x'(0)=q'}^{x'(t)=Q'} \mathcal{D}x' e^{-i\frac{\pi}{\hbar} \left( S_B[x, x'] - S_B[x', x] \right)} \bar{\rho}_B(\tilde{Q}, \tilde{Q}'; 0) \bar{\rho}_S(\tilde{q}, \tilde{q}') F[x, x'].
\] (1.34)

Equation (1.34) can be interpreted as follows. The reduced density matrices propagation consists of two sums over paths, one evolving forward in time and the other evolving backward in time. In the absence of the environment each of these paths accumulates phase independently according to the action \(S_0[q]\) which depends on the path of the system alone. However in the presence of an environment these two paths are correlated by the influence functional \(F[q, q']\), which is defined by,
\[
F[x, x'] = \int dQ \int d\tilde{Q} \int d\tilde{Q}' \int_{x(0)=Q}^{x(t)=Q} \mathcal{D}X \int_{x'(0)=Q'}^{x'(t)=Q'} \mathcal{D}X' e^{-i\frac{\pi}{\hbar} \left( S_B[x, x'] - S_B[x', x] \right)} \bar{\rho}_B(\tilde{Q}, \tilde{Q}'; 0),
\] (1.35)

So the influence functional encodes the influence of the environmental co-ordinates on these different paths. So far we have said nothing about the form of the environment (or the system), next we describe the exact expressions derived by Feynman and Vernon[33] for the case where the environment is one or many harmonic oscillators linearly coupled to a general central system.

**Influence Functional for a Single Harmonic Oscillator**

Suppose there is just one environmental coordinate, \(Q_1\), which has the action of a harmonic oscillator with mass \(m_1\) and natural frequency \(\omega_1\) and is linearly coupled
to the central system co-ordinates with a coupling \( C_1 \). That is the action for the bath is
\[
S_B[q, Q] = \int_0^t dt \left[ \frac{m_1}{2} \dot{Q}_1^2 - \frac{m_1 \omega^2}{2} Q_1^2 - \frac{C_1 \cdot q Q_1}{2} \right].
\] (1.36)

If the initial state for \( Q_1 \) is thermal, then the influence functional \( F_1[q, q'] \) is\[33\]
\[
F_1[q, q'] = \exp \left\{ -\frac{1}{\hbar} \int_0^t dt' \int_0^{t'} dt'' \left[ q(t') - q'(t') \right] \cdot \left( \text{Re}[\gamma_1(t' - t'')] \cdot \left[ q(t'') - q'(t'') \right] - i\text{Im}[\gamma_1(t' - t'')] \cdot \left[ q(t'') + q'(t'') \right] \right) \right\}
\] (1.37)
with
\[
\gamma_{1i}^{ab}(t' - t'') = \frac{C_i^a C_i^b}{2m_1 \omega_1} \left[ e^{-i\omega_1(t' - t'')} + \frac{2 \cos \omega_1 (t' - t'')}{e^{3i\omega_1} - 1} \right].
\] (1.38)

The influence functional is of form \( F_1[q, q'] = e^{i\Phi[q, q'] - \Psi[q, q']} \). The imaginary part of the exponent, \( \Phi[q, q'] \) has the form of a non-local (in time) addition to the action of the central system. While the real part of the exponent, \( \Psi[q, q'] \) decreases the contributions from paths where the density matrix is off diagonal for large periods of time.

### Multiple Harmonic Oscillators

Suppose now the bath consists of \( N_o \) (non-interacting) harmonic oscillators with co-ordinates \( \{Q_i\} \), frequencies \( \{\omega_i\} \), masses \( \{m_i\} \), and linear couplings to the central system \( C_i \). So the bath action is,
\[
S_B[q, \{Q_i\}] = \sum_i \int_0^t dt \left[ \frac{m_i}{2} \dot{Q}_i^2 - \frac{m_i \omega_i^2}{2} Q_i^2 - \frac{C_i \cdot q Q_i}{2} \right].
\] (1.39)

Then the influence functional is a product of single harmonic oscillator influence functionals\[33\],
\[
F[q, q'] = \prod_i F_i[q, q'].
\] (1.40)

When the initial state of the bath is thermal \( F_i[q, q'] \) is as in equation (1.37), with \( \gamma_1 \rightarrow \gamma_i \). Where \( \gamma_i \) is defined by equation (1.38) but with the substitutions \( \omega \rightarrow \omega_i \), \( m_1 \rightarrow m_i \) and \( C_1 \rightarrow C_i \). The full influence functional can then be conveniently described in terms of the spectral function \( J(\omega) \), defined by,
\[
J^{ab}(\omega) = \frac{\pi}{2} \sum_{i=1}^N \frac{C_i^a C_i^b}{m_i \omega_i} \delta(\omega - \omega_i).
\] (1.41)
The full influence functional is then
\[
F[q, q'] = \exp \left\{ -\frac{1}{\pi \hbar} \int_0^t dt' \int_0^{t'} dt'' \left( \mathbf{L}_2(t' - t'') \cdot (q(t'') - q'(t'')) - i \mathbf{L}_1(t' - t'') \cdot (q(t'') + q'(t'')) \right) \right\}
\]
\[
(1.42)
\]
with,
\[
\mathbf{L}_1(t) = \int_0^\infty d\omega \mathbf{J}(\omega) \sin \omega t \quad (1.43)
\]
\[
\mathbf{L}_2(t) = \int_0^\infty d\omega \mathbf{J}(\omega) \cos \omega t \coth \frac{\beta \hbar \omega}{2} \quad (1.44)
\]
So we see that as far as the dynamics of the central system are concerned, the structure of the oscillator environment can be described by a single function, the spectral density. The spectral density for a small number of oscillator modes is a sum over a small number of delta function contributions. A continuous spectral density can be obtained when there are a large number $N_o$ of oscillators, with an effectively continuous frequency spectrum. In the limit $N_o \to \infty$, for $\mathbf{J}$ to remain finite, the coupling constants $C_i$ must be of order $O(N_o^{-1/2})$.

We now briefly discuss some examples of spectral densities for different physical environments. The review article by Leggatt et al. [64] and the book by Weiss [114] as well as the references therein, give a large number of examples. If the oscillators are acoustic phonon modes in a three dimensional crystalline solid, then at low frequencies $J(\omega) \sim \omega^3$ or $\omega^5$ depending on the crystal symmetry. When the bath consists of conduction electron hole type excitations, it may be mapped to a model where the bath may be treated as an oscillator bath with a spectral density $J(\omega) \sim \omega$ for small frequencies. Optical phonons can give a a spectral density which is zero up to a specific gap frequency, then a continuos function at higher frequencies.

**Influence Functional for the Spin-Boson Problem**

The influence functional approach described above can be adapted very easily to treat a qubit coupled to an oscillator bath with a Hamiltonian of the form
\[
H = \frac{\Delta_0}{2} \tau^x + \frac{\xi_0}{2} \tau^z + \sum_{i=1}^{N} C^{ai} q_0 \tau^z Q_i + \sum_{i=1}^{N} \left( \frac{P_i^2}{2m_i} + \frac{m_i \omega_i^2 Q_i^2}{2} \right).
\]
\[
(1.45)
\]
This Hamiltonian is equivalent to the single qubit version of the spin-boson Hamiltonian (1.30), with the restriction that the interaction with the oscillator bath is in the spins $z$ component, $\Lambda_i^\mu = \hat{z}^\mu C_i q_0$ (the field $h_a$ appearing in the Hamiltonian
is of the form $\Delta_0 \hat{x} + \xi_0 \hat{z}$ in equation (1.45), any field can be put in this form so long as the interaction term only depends on $\tau^z$. The co-ordinate of the central system is then a discrete variable $q(t) = q_0 s^z(t)$, where $s^z(t) = \pm 1$. The paths which are summed over in the evolution of the central systems are specified by the times when the central spin flips. The influence functional is exactly as in equation (1.42) and can then be evaluated for each path (see [65, 114], and the references therein). When there is a traverse coupling, the problem requires some more work.

Leggett et al. describe the dynamics of the spin boson model with the Hamiltonian (1.45) and a spectral density that is a power law at low frequencies, cut off exponentially at frequencies much higher than a cut off frequency $\omega_c$. That is $J(\omega) = \eta \omega_{ph} \left( \frac{\omega}{\omega_{ph}} \right)^s e^{-\omega/\omega_c}$. They find that $\langle \tau^z(t) \rangle$ undergoes coherent under-damped oscillation for $s > 2$, there is a crossover temperature for $2 > s > 1$ where coherent under-damped oscillation gives way to over-damped decay, and a more complicated set of possible behaviours for $0 < s \leq 1$.

1.7.2 Spin Bath

A natural low energy model for localised modes interacting with the central qubits is one where the environmental modes consist of two level systems, (a “spin bath”). Supposing the bath consists of a $N$ qubits with operators $\{\sigma_i\}$ for $i = 1, \ldots, N$ then an appropriate Hamiltonian describing the central system and environment is

$$H = \sum_{a=1}^{N_S} h_a \cdot \tau_a + \sum_{a=1}^{N_S} \sum_{b \neq a}^{N_S} u_{ab}^{\mu \nu} \tau^\mu_a \tau^\nu_b + \sum_{a=1}^{N_S} \sum_{i=1}^{N} V^{\mu \alpha}_{ia} \tau^\mu_a \sigma^\alpha_i + \sum_{i=1}^{N} b_i \cdot \sigma_i + \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} v^{ij}_{\alpha \beta} \sigma^\alpha_i \sigma^\beta_j.$$ \hspace{1cm} (1.46)

This Hamiltonian is the most general Hamiltonian including local fields on the central $\{h_a\}$, bath spins $\{b_i\}$, pairwise interaction potentials among the different central spins $\{u_{ab}^{\mu \nu}\}$, bath spins $\{v^{ij}_{\alpha \beta}\}$, and between the bath spins and the central spins $\{V^{\mu \alpha}_{ia}\}$.

Of particular interest is the case where the coupling to the bath spins is not weak and the system cannot be mapped to an appropriate oscillator bath model. We will study aspects of this model in chapters 4-9.

In the following sections we will examine the relevant low energy Hamiltonian previously obtained by truncating the full Hamiltonian of a “double well” type qubit, where the two qubit states are based in two. We will see that in some cases, this Hamiltonian can include multiparty interactions not included in (1.46). We will then review some of the results previously obtained for the problem of the central spin coupled to a spin bath (the so called “central spin” problem), we will build these results on in the rest of this thesis.
Effective Qubit Systems

Consider the case where the system qubits are effective qubit system of the type discussed in section 1.2. The effective Hamiltonian of such systems can be derived using the instanton method (see [65]). When such a system is coupled to a spin bath one obtains an effective Hamiltonian for a single central qubit and its spin bath is of the form [84, 86–88, 109],

\[
H_{\text{eff}} = \Delta_0 \cos \phi_0 + \sum_j \alpha_j \cdot \sigma_j \quad + \text{h.c.} \tag{1.47}
\]

\[
+ \xi_0 \tau^z + \frac{\tau^x}{2} \sum_i \omega_i^\parallel \sigma_i^z + \frac{1}{2} \sum_i \omega_i^\perp \sigma_i^x + \sum_{i=1}^{N-1} \sum_{j=i+1}^N v_{ij}^{\alpha \beta} \sigma_i^\alpha \sigma_j^\beta \tag{1.48}
\]

In this Hamiltonian \(\Delta_0 \cos \phi_0\) is the “bare” amplitude for a central qubit to tunnel between its two levels, this may be accompanied by flips of any number of the bath spins with respect to their some axis determined by the \(\alpha_j\) vector for each bath spin. The vectors \(\{\alpha_i\}\) may have complex components representing the fact that bath spins may cause fluctuations in the tunneling probability and modify the phase accumulated on each tunneling event of the central qubit. The central qubit system has an energy difference (bias) of \(\xi_0\) between its two levels. The bath spins alignment with what we have defined as the \(z\) axis can effect the bias with a coupling constant \(\omega_j^\parallel\), so that the total bias felt by the central spin is \(\xi = \xi_0 + \sum_j \omega_j^\parallel\). The bath spins can flip (with respect to their \(z\) axis) without the influence of the central spin with amplitude \(\omega_j^\perp\). Finally there can be a small pairwise interaction \(v_{ij}^{\alpha \beta}\) between the bath spins.

Hamiltonians of the form (1.48) have been derived for the specific cases of magnetic molecule qubits [83, 84, 109] and superconducting flux qubits [87].

Prokof’ev and Stamp [86] studied this model in detail, they focused on calculating the return probability for the central spin which is initially up. This Return probability \(p_{r\uparrow}(t)\) can be defined as

\[
p_{r\uparrow}(t) \equiv \text{tr} \left[ \frac{1}{2}(1 + \tau^z)U_E(t)\frac{1}{2}(1 + \tau^x)U_E^\dagger(t) \right], \tag{1.49}
\]

where \(U_E(t)\) is the time evolution operator. Prokof’ev and Stamp found the effect of the bath on the return probability in most regimes of the model (1.48). In the regimes they studied they found tracing the bath out in such a problem could result in the motion of the central spin being averaged in a combination of four different ways. So the dynamics of the return probability are of the form

\[
p_{r\uparrow}(t) = \int d\epsilon_0 P_{\text{DB}}(\epsilon_0) \int dXP(X) \int d\phi P_{\text{Top}}(\phi) \int D\xi(t) P[\xi(t)] \int D\xi(t) P[\xi(t)] p_{r\uparrow}(t; X, \phi, \epsilon_0, \xi(t)], \tag{1.50}
\]
Here \( p_{r\varphi}(t; X, \phi, \xi_0, \xi(t)) \) is the return probability as a function of the auxiliary variables \( X, \phi, \) the initial bias \( \xi_0, \) and a functional of a time dependent bias \( \xi(t) \). The four averages each have an associated probability density function \( P(X), P_{\text{Top}}(\phi), P_{\text{DB}}(\xi_0), \) or functional \( P[\xi(t)] \). Each of these averages is associated with a distinct effect and set of terms in the Hamiltonian:

(i) **The static bias average or degeneracy blocking.** If the bath spins have no mechanism by which they can flip their \( z \) components, then the Hamiltonian reduces to \( H = \frac{1}{2} \Delta_0 \tau^z + \sum_j \omega_j^|| \sigma_j^z \) and the central qubit feels a static bias \( \hat{\xi}_0 = \hat{\xi} = \xi_0 + \sum_i \omega_i^|| \sigma_i^z \). If the bath is initialised so either, the bath is initially in a state that has an indeterminate bias \( \hat{\xi} \) (that is \( [\hat{\xi}, \rho(0)] \neq 0 \)) or measurements are performed on an ensemble of systems with different biases (e.g. the physically important case where the bath initially is in a thermal state). Then the resulting motion of the central spin will be averaged over the distribution of possible biases \( P_{\text{DB}}(\xi_0) \). This is referred to as degeneracy blocking. We discuss the dynamics in this regime in more detail in section 6.1.

(ii) **Topological decoherence.** If the main cause of the flipping of the bath spins is the tunneling term of the Hamiltonian and the bias acting on the central spin is negligible, then we will get topological decoherence. In which case the main affect of the bath spins is that they can exchange phase with the central spin every time it flips. Each time the central spin flips even numbers of bath spin may flip and averaging over the number and possible orientations of these flips (clockwise or anticlockwise) leads to decoherence. In this thesis we are mainly concerned with systems, in which this effect is negligible so we refer the reader to the references \[83, 86\] for more details on this type of decoherence.

(iii) **Precessional decoherence.** If the most important terms in the Hamiltonian which influence the dynamics of the bath spin are those with coefficients \( \omega_j^|| \) and \( \omega_j^\perp \). Then every time the central spin flips, the effective field \( \gamma_j^+ \) acting on the \( j \)’th bath spin, jumps between two distinct values, \( \gamma_j^\pm \) (illustrated in figure 1.2). This causes precessional decoherence, where the bath spin states spread out overtime as they are processing under the influence of different fields depending on what the central qubit does.

We can define an angle \( \beta_j \) for each of the bath spins \( \cos 2\beta_j = -\gamma_j^+ \cdot \gamma_j^- / (|\gamma_j^+||\gamma_j^-|) \). If \( \omega_j^|| \gg \omega_j^\perp \) then this field jumps between two almost perpendicular values and the problem is tractable, even in the non-trivial case where the coupling is strong. With the strong coupling limit in mind we plot the density of states of the possible biases on the central spin \( \sum_j \omega_j^|| \sigma_j^z \) in figure 1.3 for a case where the distribution of coupling constants \( \{\omega_j^||\} \) is sharply distributed around mean value \( \omega_0 \) (this kind of distribution is natural, for example if the bath spins share a common hyperfine
Figure 1.2: The field on the $j$’th bath spin in the precessional decoherence regime. Shown in blue we have the field acting on the bath spin when the central spin is up $\gamma_j^+$ or down $\gamma_j^-$. The angle $\beta_j$ is shaded in red.

coupling with the central spin). We see that the states are split into different polarisation groups, each with a different value for the bath $z$ polarisation $\hat{M} = \sum_j \sigma_z^j$. When this coupling is strong transitions that conserve the total interaction energies are resonant with respect to the interacting Hamiltonian and are therefore dominant. These transitions occur between polarisation groups of opposite sign (if $\xi_0$ is small compared to $\omega_0$) and a sum over possible resonant transitions leads to averaging over an auxiliary variable $X$. We will explain this in more detail in section 7.2, where we re-derive and extend the results obtained by Prokof’ev and Stamp, using a slightly different method to what they used.

(iv) Average over a dynamic bias. When the coupling $v_{ab}^{ij}$ between the bath spins is weak compared to $\omega_j^\parallel$. The interaction term has two effects: the diagonal part $v_z^{ij}$ causes further splitting of the polarisation groups (by an amount $\sim \sqrt{N}v_0$, where $v_0$ is the mean $|v_{ab}^{ij}|$), and the off diagonal parts such as $V_{xx}^{ij}$ cause pairwise flips among the bath spins which causes the bath to magnetisation to diffuse incoherently. Therefore an average over the randomly diffusing bias must be computed, we treat an example of this in section 6.3.2.

In a more general case some of these averaging effects may be combined, see [86] for more details.
Figure 1.3: The density of states of the possible biases on the central qubit in the precessional decoherence model. The shaded (blue) areas shows the density of biases in the case of a bath with a Gaussian distribution of biases around $\omega_0$. The thin (black) lines show the position of delta function contributions when all bath spins have the same coupling to the central spin.
1.8 Practical Qubits

In this chapter we discuss some practical examples of qubits, which are currently being investigated. We consider superconducting qubits, magnetic molecule based qubits, and semi-conducting spin qubits as examples.

We use superconducting qubits as an example, to show some of the various techniques which can be used to make qubits less susceptible to the influence of the environment. As such in section 1.9 we will review the basic operation of superconducting qubits, their coupling to the environment and some modern designs, which aim to minimise the effect of the environment.

In section 1.10 discuss a particular example of a magnetic molecule qubit, the Fe$_8$ qubit. We will discuss this because its spin environment and its exact coupling to the central qubit are well understood. This will allow make some concrete predictions from the theory presented later in the thesis.

Finally we will give a short discussion of semiconductor spin qubits. Because these are another experimentally relevant type of qubit, have a well understood environment, and a well developed theory to describe it.

1.9 Superconducting qubits

One of the most successful approaches to building qubits for use in quantum information systems has been to utilise superconducting electronics\[22, 23, 115, 116\]. First the basic superconducting circuit element, the Josephson junction is introduced, then the coupling of such a system to the environment is discussed, and finally three different superconducting circuit qubits are discussed: A SQUID flux qubit, a Transmon qubit, and a three Josephson junction squid qubit.

1.9.1 The Josephson Junction Circuit Element

The basic building block of most superconducting qubits are Josephson junctions \[52\] which are illustrated in figure 1.4 and consist of a layer of insulator sandwiched between two superconducting leads. The low energy dynamics of the circuit can be described in terms of the phase difference $\phi$ of the superconducting order parameter across the junction \[52\] and has the Lagrangian\[2, 52, 61\] (neglecting couplings of the pair excitations to normal electrons in the circuit, phonons, charge defects, and other modes which make up the environment)

$$L(\phi, \dot{\phi}) = \frac{\hbar^2}{4EC} \left( \dot{\phi} - \frac{Qr}{C} \right)^2 - E_J(1 - \cos \phi).$$

Which can be described by an equivalent circuit shown in figure 1.4(b). This circuit of a capacitance in parallel with a nonlinear Josephson element.
Figure 1.4: The Josephson junction circuit component. (a) The Josephson junction is made up of an insulating layer (black) separating two superconducting leads. (b) The schematic circuit element. (c) An equivalent circuit containing a capacitor in parallel with the non linear voltage current relationship.

The kinetic term in the Lagrangian is the capacitive energy of the capacitor, which depends on the energy $E_C$, which depends on $C$ the capacitance of the junction and the charge of a Cooper pair $(2e)$,$$E_C = \frac{(2e)^2}{2C}.$$ $Q_r$ is the residual charge left on the junction when the circuit is constructed. In the absence of this charge, the voltage drop $V_0$ across the junction with no current flowing through it is related to the phase difference by $\dot{\phi} = \frac{2e}{h} V_0$ [52] [105], so that the kinetic terms can be written$$\frac{\hbar^2}{4E_C} \dot{\phi}^2 = \frac{1}{2} CV_0^2.$$ (1.53) Which is the familiar expression for the energy stored on a capacitor.

The potential term $U_J = E_J(1 - \cos \phi)$ is the Josephson energy associated with the current through the junction [52] (see also [105]). The energy scale $E_J$ is related to the critical current $I_c$ (which depends on the magnitude of the superconducting order parameter and the resistance of the normal layer in the junction),$$E_J = \frac{\hbar}{2e} I_c.$$ (1.54)

We can get a Hamiltonian from the circuit Lagrangian [1.51] using the usual procedure; the canonical variable to $\phi$ is$$p_{\phi} = \frac{\partial L}{\partial \dot{\phi}} = \left( \frac{\hbar}{2e} \right)^2 C \left( \frac{\dot{\phi} - \frac{Q_r}{C}}{C} \right) = \hbar n.$$ (1.55)

$$H = p_{\phi} \dot{\phi} - L = E_C(n - n_r)^2 - E_J \cos \phi.$$ (1.56)
Here \( n_r = -Q_r/(2e) \). \( n \) can be interpreted as the net number of Cooper pairs that have crossed the junction. Now one can find the energy levels of this Hamiltonian by making the canonical substitution \( p_\phi \rightarrow -i\hbar \partial_\phi \) and solving for the eigenvalues of the Hamiltonian operator.

If the Josephson junction is wired into a circuit in such a way that there is a loop which can enclose magnetic flux \( \Phi \), an inductive term \( U_L \) must be added to the potential (and therefore the Lagrangian \( L = T - U \)),

\[
U_L = \frac{E_L}{2} (\phi - \phi_e)^2. \tag{1.57}
\]

\( E_L \) sets the scale for the inductive energy of the circuit, which depends on the enclosed magnetic flux through the circuit due an applied magnetic field \( \Phi_e \) through \( \phi_e = \frac{2e}{\hbar} \Phi_e \). \( E_L \) is set by the inductance, \( L \) of the loop

\[
E_L = \frac{\Phi_0^2}{4\pi^2 L} \tag{1.58}
\]

\[
\Phi_0 = \frac{\hbar}{2e}. \tag{1.59}
\]

\( \Phi_0 \) defines a quantum of flux and the total flux \( \Phi \) through the loop is the sum of that due to the applied field and the induced flux due to the current \( \Phi = -\frac{2e}{\hbar} (\phi_e - \phi) \). A circuit which contains a Josephson junction in a loop that encloses a magnetic flux has a Hamiltonian

\[
H = p_\phi \dot{\phi} - L = E_C(n - n_r)^2 - E_J \cos \phi + \frac{E_L}{2} (\phi - \phi_e)^2. \tag{1.60}
\]

In general to construct a qubit one wants a system of two isolated energy levels that can be excited at a specific frequency, without exciting other levels. There are several ways to achieve this; the most experimentally relevant to modern applications are discussed later in this section, but first we consider the effect of coupling a circuit containing a junction to the environment.

### 1.9.2 Coupling to the Environment

In a real system the superconducting circuit described by the Hamiltonian (1.60) will be coupled to the environment. There are several ways which the Hamiltonian (1.60) can be coupled to the environment which are particularly important when designing qubits \[22\]:

1. Charge fluctuations in the environment can lead to \( Q_r \) depending on the state of the environment resulting in time dependent charge noise.

2. Spins in the environment can cause stray magnetic fields in any inducting loops so that the applied flux \( \phi_e \) may vary with time (flux noise). So \( \phi_e \) is in general an operator on the environment.
3. The critical current $I_c$ (and therefore $E_J$) may vary due to impurities in the
junction or its coupling to phonons (critical current noise).

The different noise sources 1-3 above have the effect of promoting the variables
$Q_r$, $\phi_e$, and $I_c$ to operators acting on the environment. Fluctuations in these “noise
variables” are well characterised experimentally (see [44, 60, 71, 76, 81, 110, 125] and
the references therein). It all cases the noise is strongly peaked at low frequencies
and scales as some power of inverse frequency and is believed to be caused by fluctuating
two level systems, see [81] for a review. In the cases of charge, and critical current
noises these are thought to be because of localised electrons on defects which may
hop between different sites. This can cause fluctuations in dipole moments in the
junction, leading to a fluctuating junction resistivity and therefore a fluctuating
critical current. These localised electrons can also fluctuate the charge on a lead
and cause charge noise. The microscopic details of the couplings causing charge
noise and critical current noise are not well understood.

Experiments have shown that charge noise [76] and flux noise [44] are the key
limiting factors for coherence in the simplest qubit designs so that the more com-
plicated designs discussed below are designed around reducing these noise sources.

1.9.3 Flux Qubits

A simple flux qubit [64] for isolating two energy levels of the Hamiltonian (1.60) is
to set up the potential $U(\phi) \equiv -E_J \cos \phi + \frac{E_L}{2}(\phi - \phi_e)^2$ as in into the double well
configuration described in section 1.2. An RF-SQUID qubit is an example of this.

RF-SQUID

The simplest way to achieve a potential like that in figure 1.6 is to apply a flux
through a superconducting ring with a Josephson junction (illustrated in figure 1.5
(a)). If the flux is a half integer multiple of the flux quantum so that $\phi_e = \pi$ then the
potential $U(\phi)$ shown in figure 1.6 has the desired form, with two distinct energy
wells at $\phi = \phi_\pm$, so that a linear combination of the lowest energy level of each of the
wells form the states of the qubits. In this case ignoring the possibility of tunneling
between the two wells, each will have a ground states which we can call $|\pm 1\rangle$, with
energies $\epsilon_\pm$. Because the phase can tunnel between the wells with amplitude $\Delta_0$ the
Hamiltonian of the effective low energy qubit Hamiltonian will be

$$H = \frac{1}{2}(\epsilon_+ - \epsilon_-)\sigma^z + \Delta\sigma^x.$$ (1.61)

This type of qubit is known as a Superconducting QUantum Interference Device
(SQUID) because it is essentially a miniaturised version the device of the same
name which was used to make accurate magnetic field measurements[105]. The first
experimental demonstration of an rf-SQUID was achieved in the 60’s [50], while the
first observation of a rf-SQUID in a superposition of flux states was by Friedman et
Figure 1.5: A simple rf squid, (a) the squid consists of a superconducting ring with an insulating junction, (b) the effective circuit diagram consists of a Josephson junction and inductance as the loop can enclose flux.

Figure 1.6: The potential energy for an idealised flux qubit as a function of $\phi$ there are two minima at $\phi_{\pm}$. If we assume the two potential wells are deep, we can expand the potential around these minima and find approximate lowest energy states with energies $\epsilon_{\pm}$ in each of the minima.
al. [37]. Notably rf-SQUID qubits are used in the D-wave quantum annealing device [45, 51]. The main cause of decoherence in rf-SQUID qubits is fluctuations in the external flux [44]. There are several types of flux Qubit which are designed to reduce the coupling to the external flux. In the following section we describe one of these, 3-junction SQUID qubits.

3-Junction SQUID qubits

The 3-junction SQUID qubit first proposed by Mooij et al. [72, 79] is a flux qubit with low inductance and therefore is less sensitive to flux noise. The geometry of this qubit is shown in figure 1.7. Instead of having one Josephson junction in the SQUID there are three. Two of these (junctions one and two, say) are identical, while the third junction has an area larger by a factor of $\alpha^{-1}$ and therefore has a smaller capacitance and smaller Junction energy. In this case the three phase differences $\phi_1, \phi_2, \phi_3$ form the canonical position variables in the Lagrangian for the circuit. The parameter $\alpha$ characterises the difference between the third junction and the other two so that the Josephson energies satisfy $E_{J3} = \alpha E_{J1} = \alpha E_{J2} \equiv \alpha E_J$ (and likewise for the capacitance). The inductance is small enough that we can assume the effect of the inductive energy term is to fix the sum of the phase differences to the total external flux $\phi_1 + \phi_2 + \phi_3 = \phi_e$. Then the remaining potential term $U_J$ in the Lagrangian comes from the Josephson energies of the junctions and in terms of the variables $\phi_{\pm} = (\phi_1 \pm \phi_2)/2$ it is,

$$U_J(\phi_+, \phi_-, \phi_e) = -E_J(\alpha \cos(\phi_e - 2\phi_+) + 2 \cos \phi_+ \cos \phi_-). \quad (1.62)$$

With the parameters $\phi_e = \pi$ and $\alpha = 0.75$ the potential (1.62) is shown in figure 1.8 and has two potential wells near the origin. The states in these two wells define the low lying qubit states.

The “kinetic” term $T$ in the Lagrangian comes from the electrostatic energy on the effective capacitors. As well as the capacitances from the Josephson junction the three different superconducting “islands” can be coupled to charges in the environment; if we can treat the island between the junctions 1 and 2 as if it were grounded (we can always define voltage so that it has a zero voltage) then the effective circuit diagram for the qubit is as in figure 1.7. There are two effective “gate” capacitances $\gamma_A C$ and $\gamma_B C$ on the other islands which couple these islands to bias voltages $V_A$ and $V_B$ which depend on the state of the environment. The total kinetic term can then be written as a sum of the electrostatic energies on each of the junctions as well as the work required to charge the two gate capacitances which have charge $Q_{gA}$ and $Q_{gB}$. This gives

$$T = \frac{1}{2} C \left\{ V_1^2 + V_2^2 + \alpha(V_1 - V_2)^2 + \gamma_A V_{gA}^2 + \gamma_B V_{gB}^2 \right\} - Q_{gA} V_A - Q_{gB} V_B. \quad (1.63)$$

Using the relation between the junction voltages and phase differences, i.e., $V_j = \phi_0 \phi_j$ for $j = 1, 2$, and the relations $Q_{gA} = \gamma_A CV_{gA} = \gamma_A C(V_A - V_1)$, and $Q_{gB} = \gamma_B CV_{gB} = \gamma_B C(V_B - V_2)$, we have

$$T = \frac{1}{2} C \left\{ \phi_0^2 (\phi_1^2 + \phi_2^2 + \alpha(\phi_1 - \phi_2)^2) + \gamma_A C (V_A - V_1)^2 + \gamma_B C (V_B - V_2)^2 \right\} - \gamma_A C V_{gA} V_A - \gamma_B C V_{gB} V_B. \quad (1.64)$$
Figure 1.7: The three Josephson junction qubit proposed by Mooij *et al.*. (a) The device consists of a superconducting ring broken into three separate islands by the junctions 1, 2, and 3, junction 3 has a larger area. (b) The equivalent circuit diagram for the qubit including its capacitive coupling to external environmental voltages $V_A$ and $V_B$. 
Figure 1.8: The potential energy $U(\phi_+, \phi_-)$ from equation (1.62) with $\phi_v = \pi$ and $\alpha = 0.75$ the two minima of the two wells are marked with bullets •. States in these two wells define the two qubit states.
\[ \gamma_B C V_B = \gamma_B C (V_B - V_2) \] for the gate charges we have

\[ T = \frac{C}{2} \phi_0^2 (\dot{\phi}_1 \dot{\phi}_2) \left( 1 + \alpha + \gamma_A \right) \left( 1 + \alpha + \gamma_B \right) \left( \frac{\phi_1}{\phi_2} \right) - \frac{\gamma_A C}{2} V_A^2 - \frac{\gamma_B C}{2} V_B^2. \]  \tag{1.64}

Thus the environmental bias voltages enters only as an unimportant co-ordinate independent contribution to the Lagrangian \( L = T - U \), so that the qubit is insensitive to the bias voltages caused by charge noise.

In the original paper Mooij et al. [72] report the production and experimental results of a 3 Josephson junction qubit; unfortunately they were not able to set the flux to the optimum value and their qubit was limited by flux noise. Since then a variant of this design containing four junctions has been tested [102] and it was found that the main source factor limiting coherence is charge noise. Even more recent experiments [120] further develop the four qubit version reducing the charge noise to the point where photon shot noise from the cavity they use for read out is the main source of noise.

### 1.9.4 Transmon Qubits

This section describes the operation of the transmon qubit first presented by Koch et al. [58]. The transmon qubit is a type of charge qubit as the two states are distinguished by the charge on one side of a Josephson junction. Variants of the transmon qubit are used in Google’s [77] and IBM’s [1] prototype quantum computers. The transmon qubit has the effective circuit diagram shown in figure 1.9. It consists of SQUID ring containing two Josephson junctions shunted with a large bias capacitance \( C_B \) connected via a gate capacity with capacitance \( C_g \) to an applied gate voltage source \( V_g \). The inductance of the SQUID ring is low enough so that the flux is fixed to the applied flux and the phases across both Josephson junctions, are simply related. The effective Hamiltonian for the entire circuit reduces to

\[ H = 4E_C (n - n_g)^2 - E_J \cos \phi \]  \tag{1.65}
Here $E_C$ depends on the total effective capacitance. One can solve for the quantum energy levels by putting $n \rightarrow -i \partial_n$ and then solving for the eigenvalues $\epsilon_m(n_g, E_J, E_C)$ for $m = 0, 1, 2, \ldots$. On dimensional grounds we can write

$$\epsilon_m(n_g, E_J, E_C) = E_C E_m(n_g, E_J/E_C).$$

(1.66)

Koch et al. pointed out that when $E_J \gg E_L$ the dependence of the energy levels on the charge ($n_g$) is exponentially small. Figure 1.10 shows the lowest three energy levels of the Hamiltonian and we see it is indeed the case that the dependence of the energies on $n_g$, rapidly decreases as $E_J/E_C$ increases. Koch et al. also give a nice physical explanation for the small energy dispersion with $n_g$, which is as follows. The Hamiltonian (1.65) is identical to that of a pendulum of mass $m$, with charge $q$, and length $\ell$, under the influence of gravity and in a constant magnetic field perpendicular to the plane of the pendulum when the following identifications are made: the canonical momentum $\hbar n$ is identified with the angular momentum $L_z = L_z$, $\hbar n_g$ with $\frac{1}{2} qB\ell^2$, $E_C$ with $\frac{\hbar^2}{8m\ell^2}$, and the Josephson energy $E_J$ with the gravitational potential $mg\ell$. Thus when $E_J/E_C \gg 1$ the gravitational potential is strong, so one expects the pendulum to spend most of its time near the bottom where the potential is approximately harmonic. The magnetic field enters the Hamiltonian as a gauge field, and a change of gauge can eliminate it locally near $\phi = 0$. It is only when the pendulum rotates right around that the effect of the magnetic field is felt by the pendulum as the gauge field cannot be globally removed by a gauge change. This is when the $\phi$ variable is tunneling to another potential well at some integer multiple of $2\pi$ away so that the magnetic field enters only in the tunneling element and its magnitude can be estimated using a WKB type argument leading to a factor $\sim e^{-c\sqrt{E_J/E_C}}$ which is exponentially suppressed.
When operated with a large $E_J/E_C$ we see that the transmon qubit’s energy levels are unaffected by charge fluctuations. However if $E_J/E_C$ is too large the transmon fails to act as a qubit, as the energy gaps $\Delta E_{10} = \epsilon_1 - \epsilon_0$ and $\Delta E_{21} = \epsilon_2 - \epsilon_1$ between the ground state and the first excited state and between the first excited state and the second tend to the same value as $E_J/E_C \to \infty$, which provides an upper limit for $E_J/E_C$. Fortunately $E_J/E_C$ can be chosen to be big enough to suppress the effect of charge fluctuations while still having a significant difference between $\Delta E_{21}$ and $\Delta E_{10}$.

An additional advantage of the transmon qubit design is that its coupling to an microwave cavity allows the qubit to be controlled with microwave pulses[10], rather than using leads or gates which might host large numbers of defects which can couple to the qubit(this is what gives the transmon qubit its name it acts like a transmission line).

The first transmon qubits were constructed and tested soon after the initial proposal [48, 92]. These experiments showed that the effect of charge noise was greatly reduced compared to other charge qubits. With charge noise reduced the main cause of decoherence was the interaction of their qubits with the resonant modes of the cavity. In redesigning the cavity later experiments were able to improve the coherence time even further, and produce a qubit which is mainly limited by photon shot noise from the cavity [80, 89, 96].State of the art transmon qubits include the “X” shaped “Xmon” qubit[4, 70] and “gatemon” qubits [62, 68] where it is believed the key cause of decoherence is two level systems in the dielectric materials [68, 70].

1.10 Spin-based qubits

Another promising approach to the construction of qubits, is to use spin states in solid state systems. Here we discuss two broad classes of such qubits, spin qubits in semiconducting systems and spin qubits in insulating systems. We introduce these systems and discuss how the qubits interact with their environment.

1.10.1 Semiconducting Spin Qubits

One promising type of spin qubit, consists of either an electronic spin [75] or nuclear spin [54], of a dopant atom in a semiconductor (e.g. $^3$1P in a Silicon semiconductor[75]). These qubits are controlled by applying a voltage through a gate on the surface of the semiconductor that can effect the spin via the Zeeman effect [54]. Typically the dopant is spin$-1/2$, so that qubit levels are the spin states (although there are more complicated designs where the qubit levels are mixtures of the spin half states and other modes, see for example [63, 74]).

Typically the dominant source of environmental noise in such qubit is the nuclear spins inside the semiconductor. The effective Hamiltonian for a semiconducting
qubit spin $\tau$ coupled to the surrounding bath of nuclear spins $\{\sigma_j\}$ is\cite{5, 17, 20, 90, 121, 122}

$$H = \frac{1}{2} \Omega_z \tau^z + \frac{1}{2} \sum_j \omega_j \sigma_j^z - \frac{1}{4} \sum_j a_j \tau \cdot \sigma_j + \sum \sum H_{ij}. \hspace{1cm} (1.67)$$

$\Omega_z$ and $\omega_j$ are the Zeeman splittings for the electronic spin and nuclear spins respectively, $a_j$ is the hyperfine coupling between the nuclear and electronic spin, and $H_{ij}$ is the interaction between nuclear spins which includes, dipolar interactions.

The theory describing decoherence in these type of qubits is well developed and different to that described in 1.7.2, so we describe this briefly here for contrast. The only term in the Hamiltonian (1.67) which can flip the central spin is the off diagonal part of the hyperfine interaction $\frac{1}{4} \sum_j a_j \left( \tau^x \sigma_j^x + \tau^y \sigma_j^y \right)$. This fact is key to most sophisticated treatments of this model\cite{5, 17, 121, 122}. For example the structure of the Hamiltonian (1.68) allows the problem to be mapped (via a canonical transformation) to a relatively simple effective spin bath problem \cite{122}, with an effective Hamiltonian of the form

$$H^\text{eff} = \frac{1}{2} \sum_j \left\{ \omega_j \sigma_j^z + \sum_{i \neq j} \frac{1}{2} B_{ij} \sigma_i^+ \sigma_j^- + \sum_{i \neq j} \frac{1}{2} D_{ij} \sigma_i^z \sigma_j^z \right\} + \frac{1}{2} \tau_z \sum_j \left\{ E_j \sigma_j^z + \sum_{i \neq j} \frac{1}{2} A_{ij} \sigma_i^+ \sigma_j^- \right\} \hspace{1cm} (1.68)$$

For the parameters $A_j, B_j, D_j,$ and $E_j$ see cited references. The effective Hamiltonian (1.68) does not contain any terms that flip the central spin. So while the dynamics of the bath spin in this model may be complicated, the model is traceable and can be treated with a variety of approximations\cite{20, 67, 90, 123}. The main cause of decoherence comes from the different states of the central qubit causing the interactions between bath spins to have different strengths \cite{67}.

### 1.10.2 Insulating spin qubits

A wide variety of spin qubits in insulating systems have also been studied. From rare-earth insulators \cite{59} to crystals of single molecule magnets \cite{9, 14, 41, 100}.

These systems have an advantage when studying decoherence, in that the coupling of the qubit to the environment is relatively easy to understand. This is not the case for superconducting qubits, where most important environmental coupling comes from impurities in the superconductor and substrate. We should note that the technology required to operate a quantum information system based of single molecule magnet or rare earth spin qubits is not as developed as for superconducting qubits. Nevertheless there have been significant advances making magnetic molecule qubits which are protected from “noise” in ways analogous to the super conducting
qubits discussed earlier, see for example [97].

In general these qubits these come in regular crystalline arrays, which may have a complicated unit cell including many spins electronic spins, but at low energies they reduce to two level systems that may be described by relatively simple Hamiltonians. The qubits then couple to each other via dipolar and exchange interactions. Decoherence of the qubit causes via their coupling to collective magnon modes caused by these interactions, their coupling to phonons in the lattice, and their coupling to the bath of nuclear spins present in the sample. At low temperatures there are many situations where the dominant cause of decoherence is the spin bath.

1.11 Conclusions and Outline of the Rest of the Thesis

We discussed in section 1.5 the construction of a quantum computer, which would be a major advance of technology. We explained that for such a computer to operate the information stored in a many qubit system needs to be maintained. In sections ?? and [1.4] we saw most of the information stored in many qubits systems is contained in the multi-partite entanglements between the qubits. But until now there has been no good way quantify this multpartite entanglement. This leads to one of the key questions we seek to solve in this thesis, is there a useful way to divide up the information in a multipartite system, particularly when its parts are qubits? Chapters 2 and 3 are devoted to answering this question. In chapter 2 we show how a density matrix representing a multipartite system may be decomposed in terms of reduced density matrices on its subsystems and correlated parts, which contain the entanglement. Then in chapter 3 we apply these results to a system of qubits and show that the multipartitie entanglement is stored in correlators between components of these qubits.

In sections [1.6][1.10] of this chapter we discussed how real systems of qubits are coupled to an environment. Important questions one can ask about the effect of the environment are: how fast are the various multipartite entanglements lost to the environment? and where does the information go when it is lost “to the environment”? The remainder of the thesis is focused on these questions. We saw in sections 1.9 and 1.10 that, for many practical qubit systems, at low temperatures the environment is either a real or effective “spin bath”, which can be described as a large number of qubits. So it makes sense to study the dynamics of entanglement in qubit systems which are coupled to a spin bath. To this end, in Chapter 4 we consider the dynamics of reduced density matrix, both in a general many body system and in a system consisting of many qubits and derive a Bogoliubov-Born-Green-Kirkwood-Yvon (BBGKY) [11, 12, 56, 57, 124] type hierarchy for the equations of motion of reduced density matrices and spin correlators. This heirarchy shows how
the dynamics of different multipartite entanglements are linked. Then in chapter 5 we study the effect of formally “integrating out” an environmental spin bath from the hierarchy of equations of motion for a system of qubits. The resulting hierarchy of equations of motion are then used to study simple models of a single qubit interacting with an environmental spin bath bath in chapter 6. We see that for a simplified model, the information carried by the central system cascades into higher and higher order correlations between the central system and the bath. A complementary approach to studying qubit dynamics in a spin bath is the subject of chapter 7 where we derive the influence function in the form of what we call a “transition expansion”. We then use this method to show that this cascade of information still occurs in a more realistic model. Chapter 8 discusses the results from chapter 7 applied to a realistic model of an experimental system. Chapter 9 then studies the dynamics of highly entangled “cat states” containing large numbers of non-interacting qubits and the decay of the different correlations which diagnose entanglement is studied. Finally we present an overview the results in chapter 10.
Chapter 2
Partitioned Density Matrices and Their Correlations

In this chapter we consider the structure of the many body density matrix. We consider some general quantum system $S$ which has its degrees of freedom divided into $N$ sub-systems $\sigma_j$, with $j = 1, 2, \ldots, N$. We wish to characterise the behaviour of $S$ in terms of correlations over the $N$ sub-systems. We will show how one may describe the properties of any non-relativistic many-body quantum system $S$ in terms of a sum over all the $B_N$ different possible partitions of subsets of $S$, of functions defined for each of these partitions. Here $B_n$, for a set of $n$ distinguishable sub-systems, is the Bell number; and the functions involve various correlated and reduced density matrices defined for each different partition. We will also write this sum in terms of a complete set of entanglement correlators for the system. Having done this we will then, in the following chapter, derive a hierarchy of coupled equations of motion for these correlators.

In what follows we first define a set of correlated density matrices in terms of the full (unreduced) density matrix of the entire system $S$ we are dealing with. To make intuitively clear what these correlated density matrices are, we discuss in some detail the example of a system partitioned into 4 sub-systems. Then we give a general expression for the correlated density matrices for some part $A_n$ of the entire system containing $n$ sub-systems; and we discuss one of the key defining properties of the entanglement correlated density matrices.

2.0.1 Definition of Correlated Density Matrices

Consider a system $S$ made up of some number $N$ of distinguishable disjoint sub-systems (which we will often call “sites”, “elementary cells”, or just “cells” for short). We may then enumerate all possible different ways of partitioning $S$ into groups of subsets - this list constitutes a set $\mathcal{P}_S$. As an example, in Fig. 2.1 we show the various partitions for the case $N = 4$. We can also enumerate all possible subsets of $S$; this list forms another set $\mathcal{P}_S$.

The two sets $\mathcal{P}_S$ and $\mathcal{P}_S$ are not the same. Thus, suppose we have $N$ elementary cells. The set $\mathcal{P}_S$ of all partitions of $S$ then contains $B_N$ members, where $B_N$ is the Bell number (see for example [36]); we will label the different members by $p_\mu$, with $\mu = 1, 2, \ldots, B_N$, noting that one of the partitions $p_1$ contains only $S$ itself. The number $B_N$ grows super-exponentially with $N$ (we have $B_1 = 1, B_2 = 2, B_3 =$...).
5, \(B_4 = 15, B_5 = 52\), and already \(B_{15} \sim 1.4 \times 10^9\). We will not, need to know anything more about \(B_N\).

The set \(\mathcal{P}_S\), on the other hand, simply has as members the different subsets of \(S\); it is usually called the “power set” of \(S\). If \(S\) has \(N\) members, then the total number of members of \(\mathcal{P}_S\) is just \(2^N\); these are easily enumerated. We will sometimes label the members of \(\mathcal{P}_S\) by \(A_\alpha\), where \(a_\alpha = 1, 2, \ldots 2^N\), for a set \(S\) containing \(N\) members.

Notice that any given partition of \(S\) is made up of a specific group of subsets of \(S\) (thus, eg., the partition \((12 | 3 | 4)\) of a set \(S\) of 4 members - depicted as the 2nd of the 15 members of the partitions of this set in Fig. 2.1 - is made up of the subsets \((12), (3),\) and \((4)\) of \(S\)). We can write this statement as \(S = \bigcup_{A \in \mathcal{P}_S} A\).

With these distinctions in mind, we would like in what follows to find an expression for the total density matrix of the system in terms of all the different reduced density matrices for the different subsets of \(S\), and of all the different entanglement correlated density matrices.

We will give a precise definition of these entanglement correlated density matrices below. The reduced density matrices are defined in the usual way, i.e., we define the reduced density matrix \(\bar{\rho}_{A_\alpha}\) for some specific subset \(A_\alpha\) of \(S\) as the partial trace of the full density matrix over those other subsystem cells \(i \not\in A_\alpha\). We shall write this definition as

\[
\bar{\rho}_{A_\alpha} \equiv \operatorname{tr}_{S \setminus A_\alpha} \rho_S
\]

where \(S \setminus A_\alpha\) denotes the set containing all cells except those in the subset \(A_\alpha\); here and from now on a bar over a density matrix indicates it is a reduced density matrix.

We can then write the full density matrix in the form

\[
\rho_S = \sum_{A \subseteq S} \left( \prod_{j \not\in A} \bar{\rho}_j \right) \bar{\rho}_A^C
\]

that is, as the sum over all subsets \(A\) of \(S\) (including the sets \(\varnothing\) and \(S\)) of a “correlated part” \(\bar{\rho}_A^C\) multiplied by the reduced density matrices \(\bar{\rho}_j\) on those remaining individual cells not contained in \(A\). The above expression should be read with the following conventions:

\[
\bar{\rho}_\varnothing^C = 1 \quad \text{(2.3)}
\]

\[
\prod_{j \in \varnothing} \bar{\rho}_j = 1 \quad \text{(2.4)}
\]

\[
\bar{\rho}_i^C = 0 \quad \text{(2.5)}
\]

ie., we have that (i) the correlated part of the density matrix \(\bar{\rho}_\varnothing^C\) over a set containing no cells is 1; (ii) the product of the reduced density matrices taken over no cells is taken to be 1; and (iii) the correlated part of the density matrix for a single cell is zero. Consider, for example, some system with a number \(N > 3\) cells; and consider
the terms in the sum (2.2), in the cases where (i) $A = \emptyset$, (ii) $A = \{1, 2, 3\}$ and (iii) $A = S$. These terms are then given by

$$\rho_S = \prod_{i \in S} \bar{\rho}_i \quad (A = \emptyset) \quad (2.6)$$

$$\rho_S = \left( \prod_{i \notin \{1, 2, 3\}} \bar{\rho}_i \right) \bar{\rho}^C_{123} \quad (A = \{1, 2, 3\}) \quad (2.7)$$

$$\rho_S = \bar{\rho}^C_S \quad (A = S) \quad (2.8)$$

respectively.

There are 2 properties of the entanglement correlated parts $\bar{\rho}^C_A$ that make them useful. First, equation (2.2) is a linear expansion of the full density matrix in terms of the $\bar{\rho}^C_A$. Second, we will take it as one of the defining conditions for the entanglement correlated density matrices that if we trace any single cell out of $\bar{\rho}^C_A$ we get zero; ie., we have for any $i \in A$ that

$$\text{tr}_i \bar{\rho}^C_A = 0 \quad (\forall i \in A) \quad (2.9)$$

Now equations (2.2) and (2.9), taken together, define the correlated parts $\bar{\rho}^C_A$ uniquely. However one needs to unpack these equations to see what they really mean; and we would also like to have an explicit expression for $\bar{\rho}^C_A$. In what follows we first see how to understand (2.2) with simple examples; and we then find the desired expression for $\bar{\rho}^C_A$.

2.0.2 A 4-cell Example

The kind of thing we are talking about can be simply understood by looking at a system $S$ composed of 4 sub-systems. In what follows we do this, introducing a diagrammatic representation of the results, and showing how the expansion over entanglement correlators can also be related to one over “cumulant density matrices”.
Expansion Over Entanglement Correlators

Let us begin by looking at only 2 sub-systems (what we will call a “2-cell” system). The total density matrix $\rho^S$ for $S$ is then

$$\rho^S \equiv \rho_{12} = \bar{\rho}_1 \bar{\rho}_2 + \rho^{C}_{12} \quad (2.10)$$

where $\bar{\rho}_1$ and $\bar{\rho}_2$ are the reduced density matrices for sub-systems 1 and 2 respectively, and $\rho^{C}_{12}$ is that part of $\rho^S$ in which there are correlations between the two sub-systems. We write $\rho^S = \rho_{12}$ here to indicate the system now is just made up of two sub-systems 1 and 2.

Notice that (2.10) actually defines what we mean by $\rho^{C}_{12}$, i.e., we have defined $\rho^{C}_{12}$ as

$$\rho^{C}_{12} = \rho_{12} - \bar{\rho}_1 \bar{\rho}_2. \quad (2.11)$$

in terms of $\rho^S$, $\bar{\rho}_1$, and $\bar{\rho}_2$. The generalization of (2.10) to a 3-cell system is simple,

$$\rho_{123} = \rho^{C}_{123} + \rho^{C}_{12} \bar{\rho}_3 + \rho^{C}_{12} \bar{\rho}_3 + \rho^{C}_{12} \bar{\rho}_3 \quad (2.12)$$

A system consisting of 4 sub-systems, whose partitions were already shown in Fig. 2.1, turns out to be more interesting. Then (2.2) reads

$$\rho_{1234} = \bar{\rho}_1 \bar{\rho}_2 \bar{\rho}_3 \bar{\rho}_4 + \rho^{C}_{12} \bar{\rho}_3 \bar{\rho}_4 + \rho^{C}_{13} \bar{\rho}_2 \bar{\rho}_4 + \rho^{C}_{14} \bar{\rho}_2 \bar{\rho}_3 \quad (2.13)$$

Let us first notice how we get the lower reduced density matrices from this. We can immediately trace out cell 4, to get $\bar{\rho}_{123}$; then, because $\text{tr} \rho^{C}_{14} = \text{tr} \rho^{C}_{24} = \ldots = \text{tr} \rho^{C}_{1234} = 0$, we have

$$\bar{\rho}_{123} \equiv \text{tr}_4 \rho_{1234} \quad \text{and} \quad \rho^{C}_{123} \equiv \bar{\rho}_{123} - \bar{\rho}_1 \bar{\rho}_2 \bar{\rho}_3 + \bar{\rho}_1 \bar{\rho}_2 \bar{\rho}_3 + \bar{\rho}_1 \bar{\rho}_2 \bar{\rho}_3 \quad (2.14)$$

which is just equation (2.12) (except in the present case $\{1, 2, 3\}$ is a subset of the system so that $\bar{\rho}_{123}$ is a reduced density matrix). We can then trace out cell 3, as well, to get

$$\bar{\rho}_{12} \equiv \text{tr}_{\{3, 4\}} \rho_{1234} = \bar{\rho}_1 \bar{\rho}_2 + \rho^{C}_{12} \quad (2.15)$$

which is just equation (2.10).

Analogous expressions exist for $\rho^{C}_{23}$ and $\rho^{C}_{13}$; substituting these into expression (2.14) and rearranging we then find

$$\rho^{C}_{123} = \bar{\rho}_{123} - \bar{\rho}_1 \bar{\rho}_2 \bar{\rho}_3 - \bar{\rho}_1 \bar{\rho}_2 \bar{\rho}_3 - \bar{\rho}_1 \bar{\rho}_2 \bar{\rho}_3 + 2 \bar{\rho}_1 \bar{\rho}_2 \bar{\rho}_3. \quad (2.16)$$
so that finally we get an expression for the fourth order correlated part of the density matrix as

\[
\bar{\rho}_{1234} = \rho_{1234} - \rho_{123}^C \rho_4 - \rho_{234}^C \rho_1 - \rho_{134}^C \rho_2 - \rho_{1234}^C \rho_3
\]

\[+ \rho_{12}^C \rho_3 \rho_4 + \rho_{13}^C \rho_2 \rho_4 + \rho_{14}^C \rho_2 \rho_3 + \rho_{23}^C \rho_1 \rho_4
\]

\[+ \rho_{24}^C \rho_1 \rho_3 + \rho_{34}^C \rho_1 \rho_2 - 3 \rho_1 \rho_2 \rho_3 \rho_4. \tag{2.17}
\]

At this point it is very useful to introduce a diagrammatic representation for the various functions involved. We represent the different cells or sub-systems with “bullets” (i.e., by the symbol •), and the reduced density matrix for a group of cells is shown by linking these cells with a thick line. Then, for example, the expression \( \bar{\rho}_{134} \bar{\rho}_{2} \) is represented as shown in Fig. 2.2(a).

We now represent the entanglement correlated density matrices, like \( \bar{\rho}_{12} \), \( \bar{\rho}_{123} \), ..., by double lines linking the cells. Then, in the 4-cell example, we have for the relation between the full density matrix \( \rho_{1234} \) and the entanglement correlated density matrices \( \rho^C \), given above in (2.13), the diagrammatic representation shown in Fig. 2.3.

Before continuing with the analysis, we remark on two things about these results:

(i) we are not summing over different partitions to get these results, but over different subsets of the 4-site system, i.e., over the power set.

(ii) the number of different terms shown in Fig. 2.3 is not \( 2^4 = 16 \), as one might naively expect for the power set of our 4-site system. Instead it is \( 2^4 - 4 = 12 \). This is because the 4 subsets made from single individual sites gives no contribution - the correlated part of a single site density matrix is zero, as specified in equation (2.5). Thus in general we expect a total number of diagrams \( 2^N - N \) to contribute to the expansion (2.2).

**Expansion Over Cumulant Matrices**

As just noted, the expansion (2.2) is not an expansion over the different partitions of the total set \( S \), but over the power set. However one can also do an expansion defined directly in terms of these partitions, rather than by the zero trace condition in equation (2.9).

Suppose we take the set \( \mathcal{P}_S \) of all partitions of \( S \), and then for each one of these partitions we factorise the result into reduced density matrices for single cells uncorrelated with the rest, and a set of “cumulant reduced density matrices” \( \rho^{CC} \) for the other cells. The expansion of the total density matrix in terms of these cumulant matrices then has the same structure as a cumulant expansion of a joint probability function or functional; i.e., we can write

\[
\rho_S = \sum_{p_\mu \in \mathcal{P}_S} \prod_{A \in p_\mu} \bar{\rho}_A^{CC} . \tag{2.18}
\]
Figure 2.2: Diagrammatic representation of some of the terms in the 4-cell density matrix. In (a) we show the term $\bar{\rho}_{134}^{C} \bar{\rho}_{2}$ appearing in equation (2.17); in (b) we show the term $\bar{\rho}_{134}^{C} \bar{\rho}_{2}$, also appearing in equation (2.17); and in (c) we show the term $\bar{\rho}_{134}^{C} \bar{\rho}_{2}$, appearing in equation (2.19).

Equation (2.18) can be used to inductively to define $\bar{\rho}_{A}^{CC}$, with the convention that for a single elementary subsystem, the cumulant matrix $\bar{\rho}_{i}^{CC}$ is defined to be the reduced density matrix, i.e., $\bar{\rho}_{i}^{CC} \equiv \bar{\rho}_{i}$.

The relation between this cumulant expansion and the power set expansion we are using here, which is given in terms of entanglement correlated density matrices, is easily illustrated for the 4-cell problem, for which we find the cumulant expansion

$$\rho_{1234} = \rho_{1234}^{CC} + \rho_{123}^{CC} \rho_{4} + \rho_{124}^{CC} \rho_{3} + \rho_{134}^{CC} \rho_{2} + \rho_{234}^{CC} \rho_{1}$$

$$+ \rho_{12}^{CC} \rho_{34}^{CC} + \rho_{14}^{CC} \rho_{23}^{CC} + \rho_{13}^{CC} \rho_{24}^{CC} + \rho_{23}^{CC} \rho_{14}^{CC}$$

$$+ \rho_{13}^{CC} \rho_{24} + \rho_{14}^{CC} \rho_{23} + \rho_{12}^{CC} \rho_{34} + \rho_{24}^{CC} \rho_{13}$$

$$+ \rho_{34}^{CC} \rho_{1} \rho_{2} + \rho_{1} \rho_{2} \rho_{3} \rho_{4}$$

(2.19)

for $\rho_{1234}$ in terms of the $\rho^{CC}$.

One can of course invert the relation (2.18) as well. Thus, for example, the 4th-order cumulant density matrix is given in terms of the entanglement correlated matrices $\rho^{C}$ and the reduced density matrices by

$$\rho_{1234}^{CC} \equiv \rho_{1234}^{C} - \rho_{12}^{C} \rho_{34}^{C} - \rho_{14}^{C} \rho_{23}^{C} - \rho_{13}^{C} \rho_{24}^{C}$$

(2.20)

which when expanded out gives

$$\rho_{1234}^{CC} \equiv \rho_{1234}^{C} - \rho_{12}^{C} \rho_{34} - \rho_{14}^{C} \rho_{23} - \rho_{13}^{C} \rho_{24} - \rho_{1234}^{C} \rho_{1}$$

$$- \rho_{12}^{C} \rho_{34}^{C} - \rho_{14}^{C} \rho_{23}^{C} - \rho_{13}^{C} \rho_{24}^{C}$$

$$+ 2(\rho_{12}^{C} \rho_{34} - \rho_{13}^{C} \rho_{24} + \rho_{14}^{C} \rho_{23} - \rho_{23}^{C} \rho_{14}^{C} +$$

$$\rho_{24}^{C} \rho_{1} \rho_{3} - \rho_{34}^{C} \rho_{1} \rho_{2}) - 6 \rho_{1} \rho_{2} \rho_{3} \rho{4}.$$  

(2.21)

We can also illustrate the cumulant expansion diagramatically. If we represent the cumulant reduced density matrices $\bar{\rho}_{12}^{CC}, \ldots$ by single lines between the relevant cells (compare Figs. 2.2(b) and 2.2(c)). Then, for the relation between the full density matrix $\rho_{1234}$ and the cumulant density matrices $\rho^{CC}$, we have the diagrammatic representation shown in Fig. 2.4.

We see that the relationship between the full density matrix $\rho_{S}$ and the cumulant density matrices $\rho^{CC}$ is the same as that in a typical cumulant expansion, and so can be derived in the usual way for any value of $n$. 

2.0.3 General Properties of Entanglement Correlated Density Matrices

As we have just seen, the relationship between $\rho_S$ and the cumulant density matrices $\rho^{CC}$ is relatively straightforward. On the other hand, the relationship between $\rho_S$ and the entanglement correlated density matrices $\rho^C$ is not so obvious - we still do not have a general expression for the correlated part of the total density matrix. To properly understand things we now turn to the general case.

What we wish to show is how, for a general subset $A^{(n)}_\alpha$ of $n$ cells of a total system $S$ containing $N$ cells, the correlated part of the reduced density matrix can be written as a sum over terms involving the reduced density matrices for all subsets $C^{(m)}_\mu \subseteq A^{(n)}_\alpha$. The notation used here labels the specific subsets $C^{(m)}_\mu$ and $A^{(n)}_\alpha$ by the subscripts $\mu$ and $\alpha$; the superscripts $m$ and $n$ tell us how many cells are contained in these subsets. This is illustrated in Fig. 2.5. The key result we find can be written
Figure 2.5: A representation of the sets used in equation (2.23). The set $A_n$ is a subset of the whole system $S$, and contains $n$ members. The set $C_m$, which contains $m$ members, is a subset of $A^n$.

As

\[
\tilde{\rho}_{A_n}^{C} = \sum_{m=2}^{n} (-1)^{(n-m)} \sum_{C_{\mu}^{(m)} \subseteq A_n} \left( \tilde{\rho}_{C_{\mu}} \prod_{j \in A_n \setminus C_{\mu}} \tilde{\rho}_j \right) - (-1)^n (n-1) \prod_{j \in A_n} \tilde{\rho}_j. \tag{2.22}
\]

which says that the entanglement correlated density matrix $\tilde{\rho}_{A_n}^{C}$ for the specific set $A_n$ of cells can be written as a sum over entanglement correlated density matrices for all the different subsets $C_{\mu}^{(m)}$ of $A_n$, multiplied by the product of the reduced matrices for all the cells $j$ that are not included in the subset $C_{\mu}^{(m)}$ (this being the first term in (2.22)), minus a term which is simply the product of all the individual cell reduced density matrices for all the cells in $A_n$.

To reduce somewhat the profusion of indices in this expression, we will henceforth write expressions of this kind without the Greek indices labelling the specific subsets - thus (2.22) becomes

\[
\tilde{\rho}_{A_n}^{C} = \sum_{m=2}^{n} (-1)^{(n-m)} \sum_{C_{\mu} \subseteq A_n} \left( \tilde{\rho}_{C_{\mu}} \prod_{j \in A_n \setminus C_{\mu}} \tilde{\rho}_j \right) - (-1)^n (n-1) \prod_{j \in A_n} \tilde{\rho}_j. \tag{2.23}
\]

The simplest way to demonstrate the result in equations (2.22) and/or (2.23) is to construct an inductive proof - this is done in Appendix A. This result shows how one can define $n$-cell entanglement explicitly in terms of all possible combinations of $m$-cell entanglements over the different subsets of the $n$ cells, $\forall m < n$, along with products of single cell reduced density matrices. We shall see in the next two sections how we can employ eq. (2.23) to define a set of correlation functions which exhaustively characterise all the different kinds of entanglement that exist at the $n$th level, i., for a set of $n$ entangled cells.
As noted above, a key property of the entanglement correlation density matrices $\bar{\rho}^C$ is that any partial trace over $\bar{\rho}^C_{A_n}$ in (2.23), i.e., one in which we trace out any $i \in A_n$, gives zero - compare equation (2.9). In the discussion above, we treated this equation as a defining property of the $\bar{\rho}^C$. However, one can also derive the result explicitly from the expression (2.23). The derivation is given in Appendix A.2.

2.1 Conclusion

We have investigated the decomposition of the density matrix in a system made up of many distinguishable cells. We have defined two natural ways to decompose the system: (i) as a sum over all possible subsets of the system of terms involving entanglement correlated density matrices $\bar{\rho}^C_A$ and (ii) as a sum over all possible partitions of the system of terms which are products of cumulant density matrices $\bar{\rho}^{CC}_A$. We saw that these two decomposition are distinct when the number of cells $N \geq 4$.

In the next chapter we will discuss how in systems where the elementary cells are qubits, the reduced density matrices and different decomposition can be described in terms of correlations between different spin components. Then in chapter 4 use $\bar{\rho}^C_A$ to derive a hierarchy of equations of motion linking reduced density matrices of different sizes. We leave further exploration of the properties and uses of the cumulvent density matrices $\bar{\rho}^{CC}_A$ for future research.
Chapter 3

Structure of the Many Qubit Density Matrix

Now we consider the structure of the density matrix when the system $S$ consists of $N$ qubits. In this case, our “elementary cells” become much simpler - each cell is a single spin-$1/2$ degree of freedom. Because these cells are irreducible, ie., can no longer be split into a set of smaller “sub-cells”, we will refer in this case to the cells as “sites”.

Apart from discussing the general $N$-qubit case, we also look in detail at pairs and triplets of spins ($N = 2, 3$). The results are useful - in particular, they teach us that the easiest way to understand the hierarchy of entanglement at the level of different qubits is just to look at the different partitioned correlated density matrices.

3.1 General Results for $N$ coupled Qubits

In what follows we wish to write some of the results of the last section for a set of $N$ qubits - these results will hold regardless of what kinds of interaction may exist between the qubits, or what external fields may be acting on them.

3.1.1 Spin Representations

We begin by establishing some notation. In dealing with a set of $N$ spin-$1/2$s we write Pauli matrices for each spin as $\{\sigma^\mu_i\}$ (where $i \in \{1, 2, \ldots, N\}$ labels the site and in the “Cartesian” representation $\mu \in \{x, y, z\}$ denotes the Cartesian components). Then for a single spin we have the density matrix in the Bloch representation [31]

$$\rho = \frac{1}{2} (1 + \langle \sigma \rangle \cdot \sigma). \quad (3.1)$$

so that the purity of the density matrix is

$$tr\rho^2 = \frac{1}{2}(1 + \langle \sigma \rangle^2), \quad (3.2)$$

and for a pure state the polarization $\langle \sigma \rangle$ sits on the Bloch sphere, with $|\langle \sigma \rangle| = 1$; otherwise $|\langle \sigma \rangle| < 1$. Notice the trace

$$tr\sigma^\mu \sigma^{\nu} = 2\delta^{\mu\nu}. \quad (3.3)$$
so that the coefficient of operators in any operators Bloch expansion can be easily calculated.

In what follows we will denote the eigenstates of $\hat{\sigma}_z$ by $|\uparrow\rangle$, $|\downarrow\rangle$, so that

$$|\uparrow\rangle\langle\uparrow| = \frac{1}{2}(1 + \sigma_z) \quad (3.4)$$

$$|\downarrow\rangle\langle\downarrow| = \frac{1}{2}(1 - \sigma_z) \quad (3.5)$$

and for a pure state at some angle $\phi$ in the $xy$-plane,

$$\rho_{\sigma\sigma'} = \frac{1}{2}(|\uparrow\rangle + e^{i\phi}|\downarrow\rangle)(\langle\uparrow| + e^{-i\phi}\langle\downarrow|)$$

$$= \frac{1}{2}(1 + \cos\phi\sigma^x + \sin\phi\sigma^y). \quad (3.6)$$

with $\sigma, \sigma' = \pm 1$ labelling the rows and columns of the density matrix.

### 3.1.2 General Results for $N$ qubits

We assume a system of $N$ qubits $\{\sigma_j\}$, with $j = 1, 2, ..., N$. Let us write the density matrix for this system $\mathcal{S}$ in the form

$$\rho_\mathcal{S} = \frac{1}{2^N} \sum_{C \subseteq \mathcal{S}} \left( \prod_{i \in C} \sigma_{i}^{\mu_i} \right) \prod_{i \in C} \sigma_{i}^{\mu_i}. \quad (3.7)$$

in which the density matrix contains contributions from all $2^N$ distinct subsets $C$ of the set $\mathcal{S}$. The contribution to the density matrix from a given cluster $C$ is determined by the correlation tensor for those spins contracted into a product of the Pauli matrices then multiplied by a normalisation factor.

Clearly $\rho_\mathcal{S}$, composed entirely of Pauli matrices, must be Hermitian. The trace of $\rho_\mathcal{S}$ comes from the contribution in which $C$ is the empty set (because all the Pauli matrices are traceless) which is $2^{-N}\text{tr}(I) = 1$ as required. One can verify that $\text{tr}(\sigma_{i}^{\mu} \rho_\mathcal{S}) = \langle \sigma_{i}^{\mu} \rangle$ etc. by using the relation $\sigma_{i}^{\mu} \sigma_{i}^{\nu} = \delta^{\mu\nu} I_1 + i\epsilon^{\mu\nu\gamma} \sigma_{i}^{\gamma}$ and using the traceless property of the Pauli matrices (so that any term in the sum which contains a Pauli matrix after it has been multiplied by $\sigma_{i}^{\mu}$ gives zero). In general the density matrix must be positive semidefinite, although this is a hard condition to get a handle on using the representation (3.7), as it depends on the spectrum of $\rho_\mathcal{S}$. If $\rho_\mathcal{S}$ represents a pure state then $\rho_\mathcal{S}^2 = \rho_\mathcal{S}$, which can be used to derive those relations among the correlation functions which hold for pure states (see section 3.2.1 below for examples). More generally we have

$$\text{tr}\rho_{\mathcal{S}}^2 = \frac{1}{2^N} \sum_{C \subseteq \mathcal{S}} \left( \prod_{i \in C} \sigma_{i}^{\mu_i} \right) \left( \prod_{i \in C} \sigma_{i}^{\mu_i} \right) \leq 1. \quad (3.8)$$

As noted above, there are $2^N$ possible $C \subseteq \mathcal{S}$. When one takes the partial trace of (3.7) we see that the expression for a reduced density matrix on a set $\mathcal{A} \subset \mathcal{S}$ containing $n$ spins is of the same form as (3.7), viz.,

$$\rho_\mathcal{A} = \frac{1}{2^n} \sum_{C \subseteq \mathcal{A}} \left( \prod_{i \in C} \sigma_{i}^{\mu_i} \right) \prod_{i \in C} \sigma_{i}^{\mu_i}. \quad (3.9)$$
3.2 Some Examples

The following simple examples are useful in that they not only illustrate much of the general theory discussed so far, but they also indicate some of the ways in which it can be further developed.

3.2.1 A Pair of Qubits

Consider a pair of qubits $\sigma_1, \sigma_2$, for which the density matrix is [32]

$$\rho_{12} = \frac{1}{4} \left( 1 + \sum_{j=1,2} \langle \sigma_j \mu \rangle \sigma_j \mu + \langle \sigma_1 \mu \sigma_2 \nu \rangle \sigma_1 \mu \sigma_2 \nu \right)$$

(3.10)

We can split this up to a correlated and uncorrelated part, according to

$$\rho_{12} = \rho_1 \rho_2 + \rho_{12}^C$$

$$= \frac{1}{4} \prod_j \left( 1 + \langle \sigma_j \mu \rangle \sigma_j \mu \right) + \frac{1}{4} \langle \langle \sigma_1 \mu \sigma_2 \nu \rangle \rangle \sigma_1 \mu \sigma_2 \nu$$

(3.11)

where we have defined

$$\langle \langle \sigma_1 \mu \sigma_2 \nu \rangle \rangle = \langle \sigma_1 \mu \sigma_2 \nu \rangle - \langle \sigma_1 \mu \rangle \langle \sigma_2 \nu \rangle.$$

(3.12)

Now $\rho_{12}$ is a $4 \times 4$ hermitian matrix with unit trace, and as such has 16-1=15 free real parameters, viz., 3 components of $\langle \sigma_1 \rangle$ and $\langle \sigma_2 \rangle$ each, and 9 components of $\langle \sigma_1 \mu \sigma_2 \nu \rangle$. In the case of a single qubit in a pure state, the spin had to lie on the Bloch sphere. In the two-qubit case things are more complicated; for a pure state one requires $\rho_{12}^2 = \rho_{12}$, which leads to the following constraints on the correlators,

$$3 = \langle \sigma_1 \rangle^2 + \langle \sigma_2 \rangle^2 + \langle \sigma_1 \mu \sigma_2 \nu \rangle \langle \sigma_1 \mu \sigma_2 \nu \rangle$$

(3.13)

$$\langle \sigma_1 \mu \rangle = \langle \sigma_1 \mu \sigma_2 \beta \rangle \langle \sigma_2 \beta \rangle$$

(3.14)

$$\langle \sigma_2 \beta \rangle = \langle \sigma_1 \alpha \mu \rangle \langle \sigma_1 \alpha \beta \rangle$$

(3.15)

$$\langle \sigma_1 \mu \sigma_2 \nu \rangle = \langle \sigma_1 \mu \rangle \langle \sigma_2 \nu \rangle - \frac{1}{2} \varepsilon^{\mu \alpha \lambda} \varepsilon^{\nu \beta \gamma} \langle \sigma_1 \alpha \lambda \sigma_2 \gamma \rangle \langle \sigma_1 \lambda \sigma_2 \gamma \rangle.$$  

(3.16)

This gives $1 + 3 + 3 + 9 = 16$ constraint equations on the correlators for a pure state - obviously only 10 of these are independent, since there is a 6-dimensional set of real numbers which describes the possible pure states (8 real numbers describe a 2-qubit ket $|\psi\rangle$, reduced by two by the requirements of normalization and the invariance of $\rho_{12} = |\psi\rangle \langle \psi |$ under phase rotations). For the pure state,

$$|\psi\rangle = \sum_{\sigma \sigma'} a_{\sigma \sigma'} e^{i \phi_{\sigma \sigma'}} |\sigma \sigma'\rangle$$

(3.17)

where $\sigma, \sigma' = |\uparrow\rangle, |\downarrow\rangle$; the normalization condition is then $\sum_{\sigma \sigma'} a_{\sigma \sigma'}^2 = 1$. 

For a general mixed state of two qubits, equations (3.13-3.16) are replaced by a set of three independent inequalities, which ensure the positivity of the density matrix[38]. This reflects the fact that a mixed state density matrix requires 15 independent real parameters (the 16 required to define an arbitrary $4 \times 4$ hermitian matrix, minus one because the matrix must be traceless) rather than the eight required to define a pure state.

Of particular interest for qubit pairs are “cat states”, which are fully entangled. An example of such a state is $|\Psi_C^2\rangle$, with wave-function and density matrix given by

$$|\Psi_C^2\rangle \equiv \frac{1}{\sqrt{2}} \left( |\uparrow\uparrow\rangle + e^{i\phi_{\downarrow\downarrow}} |\downarrow\downarrow\rangle \right)$$

$$|\Psi_C^2\rangle\langle\Psi_C^2| = \frac{1}{4} \left( 1 + \cos \phi_{\downarrow\downarrow} \left[ \sigma^x_1 \sigma^x_2 - \sigma^y_1 \sigma^y_2 \right] 
+ \sin \phi_{\downarrow\downarrow} \left[ \sigma^y_1 \sigma^x_2 + \sigma^x_1 \sigma^y_2 \right] + \sigma^z_1 \sigma^z_2 \right)$$  \hspace{1cm} (3.19)

When we come to look at entanglement dynamics, it is then the correlated part of these functions which will interest us.

Let us now consider the relationship between $\rho_{12}^C$ and the different types of entanglement. There is some subtlety in this [47], especially in the case of mixed states. Consider, for instance, a mixed state which is an incoherent mixture of the state $|\uparrow\uparrow\rangle$, with spins are polarised in the $z$ direction, and the state $|\rightarrow\rightarrow\rangle$, with both spins polarised in the $x$ direction, so that

$$\rho_{12} = \frac{1}{2} \left( |\uparrow\uparrow\rangle\langle\uparrow\uparrow| + |\rightarrow\rightarrow\rangle\langle\rightarrow\rightarrow| \right)$$

$$= \frac{1}{4} \left[ 1 + \frac{1}{2} (\hat{x} + \hat{z}) \cdot (\hat{\sigma}_1 + \hat{\sigma}_2) + \frac{1}{2} (\sigma^x_1 \sigma^x_2 + \sigma^y_1 \sigma^y_2 + \sigma^z_1 \sigma^z_2) \right] .$$  \hspace{1cm} (3.20)

Now $\rho_{12}$ has non-zero correlation functions; we have

$$\langle\langle \sigma^x_1 \sigma^x_2 \rangle \rangle = \langle\langle \sigma^y_1 \sigma^y_2 \rangle \rangle = \langle\langle \sigma^z_1 \sigma^z_2 \rangle \rangle = \frac{1}{4} .$$  \hspace{1cm} (3.21)

On the other hand, since $\rho_{12}$ is an incoherent mixture of two separable states, it has zero entanglement of formation[8]. This is not the only measure of entanglement; and for a general mixed state the formulae for different entanglement measures may be quite complicated.

This example shows nicely that it makes sense to consider directly the set of correlators, instead of the different entanglement measures. Because the full set of 15 correlators completely specifies the density matrix, all information about entanglement between the pair of qubits is then contained in these correlators. Since any entanglement witness [43, 46, 104] used to detect entanglement is necessarily a Hermitian operator, it follows that its expectation can also be written as a weighted sum over the correlators. Thus we can simply use the correlators themselves as the primary quantities, whose behaviour is to be determined.
### 3.2.2 Three Qubits

For a system with three qubits, the general density matrix is written as a sum over correlators as

\[ \rho_{123} = \frac{1}{8} \left( 1 + \sum_j \langle \sigma_{1\mu} \rangle \sigma_j^\mu + \sum_{i<j} \langle \sigma_{i\mu} \sigma_{j\nu} \rangle \sigma_i^\mu \sigma_j^\nu + \langle \sigma_{1\mu} \sigma_{2\nu} \sigma_{3\lambda} \rangle \sigma_1^\mu \sigma_2^\nu \sigma_3^\lambda \right) \]  

(3.22)

We now have a number of different types of entangled state. Consider as an example the three different states

\[ |\Psi_a^3\rangle = \frac{1}{\sqrt{2}} (|\uparrow\uparrow\downarrow\rangle + |\downarrow\downarrow\downarrow\rangle) \]  

(3.23)

\[ |\Psi_b^3\rangle = \frac{1}{\sqrt{2}} (|\uparrow\uparrow\uparrow\rangle + |\downarrow\downarrow\downarrow\rangle) \]  

(3.24)

and

\[ |\Psi_c^3\rangle = \frac{1}{\sqrt{3}} \sum_{\sigma_1,\sigma_2,\sigma_3} |\sigma_1\sigma_2\sigma_3\rangle \delta[\sum_j \sigma_j + 1] \]

\[ = \frac{1}{\sqrt{3}} (|\uparrow\downarrow\downarrow\rangle + |\downarrow\uparrow\downarrow\rangle + |\downarrow\downarrow\uparrow\rangle) \]  

(3.25)

For each of these states we can find the non-zero expectation values for the correlators in the density matrix representation (3.22). Consider first |\Psi_a^3\rangle, for which

\[ \langle \sigma_z^1 \sigma_z^2 \rangle = \langle \sigma_z^1 \sigma_z^3 \rangle = \langle \sigma_z^2 \sigma_z^3 \rangle = -\frac{1}{2} \]

\[ \langle \sigma_x^1 \sigma_x^2 \rangle = \langle \sigma_x^1 \sigma_x^3 \rangle = \langle \sigma_x^2 \sigma_x^3 \rangle = 1 \]  

(3.26)

We that |\Psi_a^3\rangle does not have 3-qubit entanglement, because we can write |\Psi_a^3\rangle = \frac{1}{\sqrt{2}} (|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle) \otimes |\uparrow\rangle, and this is reflected in the fact that the correlated part of the three point function, \langle \langle \sigma_t^1 \sigma_z^2 \sigma_z^3 \rangle \rangle defined by

\[ \langle \langle \sigma_t^1 \sigma_z^2 \sigma_z^3 \rangle \rangle = \text{tr} \left( \sigma_t^1 \sigma_z^2 \sigma_z^3 \rho_{123}^C \right) \]

\[ = \langle \langle \sigma_t^1 \sigma_z^2 \sigma_z^3 \rangle \rangle - \langle \sigma_t^1 \sigma_z^2 \sigma_z^3 \rangle - \langle \sigma_t^1 \sigma_z^2 \sigma_z^3 \rangle - \langle \sigma_t^1 \sigma_z^2 \sigma_z^3 \rangle \]  

(3.27)

is zero. However it does have 2-qubit entanglement and single qubit polarization.

Now consider the other two states, for which we have

\[ |\Psi_b^3\rangle : \langle \sigma_t^1 \sigma_z^2 \rangle = \langle \sigma_t^1 \sigma_z^3 \rangle = \langle \sigma_z^1 \sigma_z^3 \rangle = \langle \sigma_t^2 \sigma_z^3 \rangle = 1 \]

\[ \langle \sigma_t^1 \sigma_z^2 \sigma_z^3 \rangle = \langle \sigma_t^1 \sigma_z^2 \sigma_z^3 \rangle = \langle \sigma_t^1 \sigma_z^2 \sigma_z^3 \rangle = -1 \]  

(3.28)

For each of these states we can find the non-zero expectation values for the correlators in the density matrix representation (3.22). Consider first |\Psi_a^3\rangle, for which

\[ \langle \sigma_z^1 \sigma_z^2 \rangle = \langle \sigma_z^1 \sigma_z^3 \rangle = \langle \sigma_z^2 \sigma_z^3 \rangle = -\frac{1}{2} \]

\[ \langle \sigma_x^1 \sigma_x^2 \rangle = \langle \sigma_x^1 \sigma_x^3 \rangle = \langle \sigma_x^2 \sigma_x^3 \rangle = 1 \]  

(3.29)
for the second state, and
\[
|\Psi_c^3\rangle : \quad \langle \sigma_i^x \rangle = \langle \sigma_i^x \sigma_j^x \rangle = \frac{-1}{3}, \quad \langle \sigma_i^y \sigma_j^y \rangle = \frac{2}{3},
\]
\[
\langle \sigma_i^z \sigma_j^z \rangle = 1, \quad \langle \sigma_i^y \sigma_j^y \sigma_\ell^z \rangle = \frac{2}{3},
\]
(for \(i, j, \ell\) distinct \(\in \{1, 2, 3\}\)).

for the third state. Both \(|\Psi_b^3\rangle\) and \(|\Psi_c^3\rangle\) do have three qubit entanglement, as the correlated 3-qubit functions are non-zero (this especially obvious in the case of \(|\Psi_b^3\rangle\), which is the superposition of two terms, each of which is obtained from a triple spin flip of the other). Both states also have 2-qubit entanglement, and \(|\Psi_c^3\rangle\) also has single qubit polarisation. It can be shown that the states \(|\Psi_b^3\rangle\) and \(|\Psi_c^3\rangle\) are members of the only two different classes of fully entangled 3-qubit states [28], and all other fully entangled states can be obtained from them by local operations assisted with classical communication.

We observe that neither of the states \(|\Psi_b^3\rangle\), \(|\Psi_c^3\rangle\) has a full “3-qubit entanglement” in the way that \(|\Psi_C^2\rangle\) has full “2-qubit entanglement”. For \(|\Psi_C^2\rangle\) all the single qubit correlators are zero, whereas for the 3-qubit system it is impossible for the following three conditions to hold at once:

\[
\langle \sigma_i^\mu \rangle = 0 \quad \forall i \in \{1, 2, 3\} \quad (3.31)
\]
\[
\langle \sigma_i^\mu \sigma_j^\nu \rangle = 0 \quad \forall i \neq j \in \{1, 2, 3\} \quad (3.32)
\]
\[
\rho_{123} \text{ represents a pure state.} \quad (3.33)
\]

To show this, we note that the first two conditions imply \(\rho_{123} = \frac{1}{8} (I + \langle \sigma_1^\mu \sigma_2^\nu \sigma_3^\lambda \rangle \sigma_1^\mu \sigma_2^\nu \sigma_3^\lambda \rangle)\). We can then calculate \(\rho_{123}^2\) and we find that the \(\sigma_1^\mu \sigma_2^\nu \sigma_3^\lambda\) component is

\[
\frac{1}{32} \langle \sigma_1^\mu \sigma_2^\nu \sigma_3^\lambda \rangle \sigma_1^\mu \sigma_2^\nu \sigma_3^\lambda \neq \frac{1}{8} \langle \sigma_1^\mu \sigma_2^\nu \sigma_3^\lambda \rangle \sigma_1^\mu \sigma_2^\nu \sigma_3^\lambda \quad (3.34)
\]

where the inequality \(\neq\) holds for any non-zero value of \(\langle \sigma_1^\mu \sigma_2^\nu \sigma_3^\lambda \rangle\). Thus the state can’t be pure.

### 3.2.3 N-qubit states

There are still simple questions one can ask about \(N\)-qubit states; for example, whether an analogue of the statements (3.31,3.33) be true when we have \(N\) qubits. In other words, one can ask: does the \(N\)-qubit density matrix

\[
\rho_{12...N} = \frac{1}{2^N} \left( I + \langle \sigma_1^{\mu_1} \sigma_2^{\mu_2} \ldots \sigma_N^{\mu_N} \rangle \sigma_1^{\mu_1} \sigma_2^{\mu_2} \ldots \sigma_N^{\mu_N} \rangle \right) \quad (3.35)
\]

represent a valid pure state? The answer is that this is true only if \(N = 1\) or \(N = 2\). For \(N = 3\) we have just seen that is not a pure state, and proofs for the non-existence of pure states of the form (3.35) for \(N \geq 4\) are given in the literature ([49], and refs therein).
N-qubit Cat States

Consider the class of $N$ spin cat states,

$$|\psi^N_c(\phi)\rangle = \frac{1}{\sqrt{2}} \left( |\uparrow\uparrow\ldots\uparrow\rangle + e^{i\phi} |\downarrow\downarrow\ldots\downarrow\rangle \right)$$

$$|\psi^N_c(\phi)\rangle\langle\psi^N_c(\phi)| = \frac{1}{2} \left( |\uparrow\uparrow\ldots\uparrow\rangle\langle\uparrow\uparrow\ldots\uparrow| + |\downarrow\downarrow\ldots\downarrow\rangle\langle\downarrow\downarrow\ldots\downarrow| + e^{-i\phi} |\uparrow\uparrow\ldots\uparrow\rangle\langle\downarrow\downarrow\ldots\downarrow| + e^{i\phi} |\downarrow\downarrow\ldots\downarrow\rangle\langle\uparrow\uparrow\ldots\uparrow| \right).$$

Here $\phi$ is an angle which specifies the phase difference between the two superimposed states. We will consider the dynamics of these states and their generalisations in chapter 9. These are highly entangled states that posses many body entanglement [43]. In the Bloch vector representation (sums over sets here include a zero set term),

$$|\uparrow\uparrow\ldots\uparrow\rangle\langle\uparrow\uparrow\ldots\uparrow| = \frac{1}{2^N} \sum_{C \subseteq S} \prod_{i \in C} \sigma^z_i$$

$$|\downarrow\downarrow\ldots\downarrow\rangle\langle\downarrow\downarrow\ldots\downarrow| = \frac{1}{2^N} \sum_{C \subseteq S} \prod_{i \in C} (-\sigma^z_i)$$

$$|\uparrow\uparrow\ldots\uparrow\rangle\langle\downarrow\downarrow\ldots\downarrow| = \prod_{i \in C} |\uparrow_i\rangle\langle\downarrow_i| = \prod_{i \in C} S^+_i = \frac{1}{2^N} \prod_{S} (\sigma^x_i + i\sigma^y_i).$$

So the only non zero correlators containing $x$ and $y$ spin components in the density matrix are those of the form $\langle \prod_{C} \sigma^x_i \prod_{S \setminus C} \sigma^y_i \rangle$ (i.e. they contain correlation between components all qubits in the cat state) and one has

$$|\psi^N_c(\phi)\rangle\langle\psi^N_c(\phi)| = \frac{1}{2^N} \left\{ \sum_{C \subseteq S} \prod_{i \in C} \sigma^z_i + \sum_{C \subseteq S} \cos \left( \phi + \frac{\pi|C|}{2} \right) \prod_{S \setminus C} \sigma^x_i \prod_{C} \sigma^y_i \right\}.$$ (3.41)

The genuine $N$-partite entanglement of this state manifests itself in the order $N$ off diagonal correlators. One could also consider a generalised cat state which is conveniently described using the vector $\bar{s} = (s_1, s_2, \ldots, s_N)$ where all $s_i = \pm 1$ define

$$|\psi^N_{c\bar{s}}(\phi)\rangle \equiv \frac{1}{\sqrt{2}} \left( |\bar{s}\rangle + e^{i\phi} |\bar{s}\rangle \right)$$ (3.42)
we have

\[ | \uparrow \cdots \uparrow \rangle \langle \uparrow \cdots \uparrow | = \frac{1}{2^N} \sum_{C \subseteq S} \prod_{i \in C} s_i \sigma^z_i \]  \hspace{1cm} (3.43)

\[ | \downarrow \cdots \downarrow \rangle \langle \downarrow \cdots \downarrow | = \frac{1}{2^N} \sum_{C \subseteq S} \prod_{i \in C} (-s_i \sigma^z_i) \]  \hspace{1cm} (3.44)

\[ | \uparrow \cdots \uparrow \rangle \langle \downarrow \cdots \downarrow | = \prod_{i \in C} |s_i\rangle \langle -s_i| = \frac{1}{2^N} \prod_{S \setminus C} \sigma^x_i \prod_{C} s_i \sigma^y_i \]  \hspace{1cm} (3.45)

\[ |\psi^N_{cs}(\phi)\rangle \langle \psi^N_{cs}(\phi)| = \frac{1}{2^N} \left\{ \sum_{C \subseteq S} \prod_{i \in C} s_i \sigma^z_i + \sum_{C \subseteq S} \cos \left( \phi + \frac{\pi |C|}{2} \right) \prod_{S \setminus C} \sigma^x_i \prod_{C} s_i \sigma^y_i \right\}. \]  \hspace{1cm} (3.46)

Since \( N = 4 \) is the smallest number of qubits for which \( \rho^C_S \) is distinct from \( \rho^{CC}_S \), it is instructive to compute these two quantities for the cat state. For the generalised cat state (3.46) with \( N = 4 \) we have

\[ \rho^{C}_{1234} = \frac{1}{16} \left\{ \sum_{C \subseteq S} \cos \left( \phi + \frac{\pi |C|}{2} \right) \prod_{S \setminus C} \sigma^x_i \prod_{C} s_i \sigma^y_i + s_1 s_2 s_3 s_4 \sigma^x_1 \sigma^y_2 \sigma^z_3 \sigma^z_4 \right\} \]  \hspace{1cm} (3.47)

\[ -3 \sum_{i=1}^{3} \sum_{j>i} s_i s_j \sigma^x_i \sigma^z_j \}

\[ \rho^{CC}_{1234} = \frac{1}{16} \left\{ \sum_{C \subseteq S} \cos \left( \phi + \frac{\pi |C|}{2} \right) \prod_{S \setminus C} \sigma^x_i \prod_{C} s_i \sigma^y_i - 2 s_1 s_2 s_3 s_4 \sigma^x_1 \sigma^y_2 \sigma^z_3 \sigma^z_4 \right\} \]  \hspace{1cm} (3.48)

\[ -3 \sum_{i=1}^{3} \sum_{j>i} s_i s_j \sigma^x_i \sigma^z_j \}

3.3 Conclusion

We have seen how the density matrix in a system of many qubits can be decomposed in terms of correlations between different spin components of all the possible clusters of qubits. We have then discussed examples of states in systems of qubits, focusing on the complicated relationship between the different types of entanglement and these correlators.

When we deal with the full complexity of \( N \)-qubit states, it is hard to get very far in the analysis of entanglement, beyond simple statements of the kind presented here. The number of possible partitions of the system becomes immense, growing super-exponentially as the Bell number, and to characterise the entanglement properties
is clearly going to be very complicated. There is a large body of literature on the
different types of multipartite entanglement, along with several reviews [43, 47, 113].

However, again, even for $N$ spins, any observable witness we build to diagnose
this entanglement can be expressed as a sum of different clusters of Pauli operators.
Thus again it makes sense to go back to the study the dynamics of these correlators,
in order to understand the dynamics of entanglement - this is perhaps the main
lesson of the examples just examined.

The remainder of this thesis is therefor devoted to studying the dynamics of
these correlators in many qubit systems.
Chapter 4

Dynamics of Partitioned Density Matrices

One of our main objectives is to derive the dynamics of the entanglement correlated density matrices. For a system $S$ made up from $N$ sub-systems or “cells”, this means finding the equations of motion for each of the reduced density operators $\bar{\rho}_A$, as well as the correlated density operators $\bar{\rho}_C^A$, which describe the different sub-sets $A$ of $S$. Now, unless the Hamiltonian for $S$ is trivially non-interacting (i.e., it consists of a simple sum of terms over each cell, with no interactions between the cells), it is clear that these equations of motion will actually couple the different $\bar{\rho}_C^A$, since any sub-set $A$ will have interactions with cells not contained in that sub-set (unless of course $A = S$). Thus we will end up with set of coupled equations of motion, which takes the form of a hierarchy of coupled differential equations.

In what follows we begin by deriving the hierarchy for a general closed system in which all interactions between the different cell subsystems are pairwise. Then, in order to see how things look for a specific example, we derive the hierarchy for the system of $N$ qubits discussed in the previous section, with a set of local fields on each qubit as well as pairwise interactions between them.

4.1 Result for $N$-partite System

In the most common kind of Hamiltonian in physics, one has (i) a “free” or trivial part which only acts inside individual cells, along with (ii) an interacting part which contains pairwise terms between cells. The Hamiltonian then takes the form

$$H_S \equiv H_S^0 + H_S^I = \sum_{j \in S} \left( H_i^0 + \frac{1}{2} \sum_{i \neq j \in S} V_{ij} \right) \quad (4.1)$$

We make no assumptions for the moment about the nature of the cells, or of the interactions between them, except those assumptions already noted in the Introduction, viz., that we refer to distinguishable sets of degrees of freedom for each cell (so that there are no “exchange terms” between cells), and the system is assumed non-relativistic.

The equation of motion for the system density matrix is

$$i\hbar \partial_t \rho_S = [H_S, \rho_S]. \quad (4.2)$$
Starting from this equation, and taking its trace over all cells except those contained in $A_n$, one can derive an equation of motion for the reduced density matrix $\bar{\rho}_{A_n}$ which takes the form

$$i\hbar \partial_t \bar{\rho}_{A_n} = \left[ \bar{H}_{A_n}, \bar{\rho}_{A_n} \right] + \sum_{\ell \notin A_n} \text{tr} \left( \sum_{j \in A_n} \left[ V_{j,\ell}, \bar{\rho}_{A_n \cup \{\ell}\}} \right] \right).$$

(4.3)

where we have defined an effective local Hamiltonian (ie., one entirely restricted to $A_n$), by

$$\bar{H}_{A_n} = \sum_{j \in A_n} \left( H_0^j + \frac{1}{2} \sum_{i \neq j \in A_n} V_{ij} \right) \quad (4.4)$$

Although equation (4.3) apparently has a fairly simple form, its derivation is actually quite lengthy, and we have found no way to shorten it. This derivation appears in appendix B.1.

We can interpret (4.3) by noting first that the time evolution of $\bar{\rho}_{A_n}$ is determined both by the local Hamiltonian $H_{A_n}$, acting solely on $A_n$, and by the effect of interactions on all possible sets containing $A_n$ along with one other member.

One can think of the local effective Hamiltonian as one in which all interaction terms act solely on pairs of cells within $A_n$, ie., it is an “internal” effective Hamiltonian for $A_n$. The second “interaction” term in (4.3) is then one in which $V_{j,\ell}$ couples $\bar{\rho}_{A_n}$ to “larger” reduced density matrices $\bar{\rho}_{A_n \cup \{\ell}\}}$ which involve not only all the cells in $A_n$ but also one other cell $\ell$ from $S$ that is outside $A_n$; we then sum over all the different cells $\{\ell\}$ that are outside $A_n$. That there is only one other cell involved follows because we have only pairwise interactions in the original Hamiltonian.

To see how this works let us consider a simple example. Suppose one has an $N$-cell system $S$, and we define a specific sub-set $A^{(n)}_\alpha$ of $S$ by removing 4 designated cells from $S$ (so that $n = N - 4$). This example is illustrated in Fig. 4.1. Writing out the sum over $\ell$ in equation (4.3) explicitly we have (omitting the subscripts on the set variables),

$$i\hbar \partial_t \bar{\rho}_A = \left[ \bar{H}_A, \bar{\rho}_A \right] + \sum_{j \in A} \left( \text{tr} \left[ V_{j,1}, \bar{\rho}_{A \cup \{1\}} \right] + \frac{1}{2} \text{tr} \left[ V_{j,2}, \bar{\rho}_{A \cup \{2\}} \right] \right)$$

$$+ \text{tr} \left[ V_{j,3}, \bar{\rho}_{A \cup \{3\}} \right] + \text{tr} \left[ V_{j,4}, \bar{\rho}_{A \cup \{4\}} \right] \right);$$

(4.5)

and we see explicitly how the equation of motion for the $(N - 4)$-cell system $A^{(n)}_\alpha$ involves a coupling between the $(N-4)$-cell density matrix $\rho_{A^{(n)}_\alpha}$ and a set of $(N-3)$-cell density matrices $\bar{\rho}_{A^{(n)}_\alpha \cup \{\ell\}}$, with $\ell = 1, 2...4$.

In the next sub-section we discuss the example of a system of qubits; this will allow us to work out expressions like this explicitly.
Figure 4.1: An illustration of the terms in the sum in equation (4.5). The set $\mathcal{A}$, a subset of the total system $\mathcal{S}$, is shown in blue in (a), along with four other sets 1, 2, 3, 4 distinct from $\mathcal{A}$. Then in (b) in green we show the four different sets that can be made from the union of $\mathcal{A}$ and one of the other sets. Each dotted line represents a possible term in the sum (4.5) due to an interaction potential. We have omitted the subscripts on the set variables.

As already noted above, there is a loose analogy here with the Schwinger-Dyson equations in quantum field theory and in non-relativistic many-body theory, in that we end up with a chain of coupled integro-differential equations for the $\bar{\rho}_{\mathcal{A}^{(n)}}$ (here we restore the indices $\alpha$ and $n$, to emphasise that we are dealing in all these equations with a specific subset of $\mathcal{S}$ in which $n$ denotes the number of cells involved, and $\alpha$ the specific set of $n$ cells that has been chosen).

4.2 Hierarchy of Equations for Reduced Density Matrices $N$ Qubits

For our set of $N$ qubits, the $\{\sigma_i\}$, the cells again become individual sites, each with its own qubit. We wish to find the dynamics of the various spin correlators, following the general theory given in section 4.1. For this we need a Hamiltonian for the $N$-qubit system. The general pairwise interaction Hamiltonian for this case is:

$$H = \sum_i \frac{1}{2} h_i \cdot \sigma_i + \sum_{i=1}^{N-1} \sum_{j<i} \frac{1}{2} V_{ij}^{\mu\nu} \sigma_i^\mu \sigma_j^\nu.$$  (4.6)

In this Hamiltonian each qubit feels a local field $h_j$, and we have a pairwise interaction $V_{ij}^{\mu\nu}$ between the qubits. Commonly used examples are (i) the quan-
tum Ising model, for which \( h_i = h_0 \sigma^x_i \) and \( V_{ij}^{\mu \nu} \sigma_i^{\mu} \sigma_j^{\nu} = V_{ij}^{zz} \delta^{\mu z} \delta^{\nu z} \), and (ii) the nearest-neighbour Heisenberg model, where \( h_i = h \) is a uniform external field, and \( V_{ij}^{\mu \nu} \sigma_i^{\mu} \sigma_j^{\nu} = J_o \delta^{\mu \nu} \), with \( i, j \) restricted to be nearest neighbours.

In what follows we first derive the general hierarchy of equations of motion, and then look at some simple special cases.

### 4.2 General Form of Hierarchy

We derive the equations of motion for the various spin correlators from the reduced density matrix equation of motion we have found in (4.3). Again, we pick a specific subset \( \mathcal{A} \) of the total \( N \)-qubit system; we will therefore be interested in the time evolution of expectation values of products of spin operators for spins in \( \mathcal{A} \).

The result of the calculation can be read off from the general equation of motion in (4.3); the commutators are evaluated in Appendix B.2, and we find

\[
\frac{d}{dt} \langle \prod_{i \in \mathcal{A}} \sigma_i^{\mu_i} \rangle = \sum_{i \in \mathcal{A}} \varepsilon^{\mu \alpha \nu} h_i^\alpha \langle \sigma_i^{\nu} \prod_{j \in \mathcal{A} \setminus \{i\}} \sigma_j^{\mu_j} \rangle + \sum_{i \in \mathcal{A}} \sum_{j \in \mathcal{A} \setminus \{i\}} \varepsilon^{\mu \alpha \nu} V_{ij}^{\alpha \mu} \langle \sigma_i^{\nu} \prod_{k \in \mathcal{A} \setminus \{i, j\}} \sigma_k^{\mu_k} \rangle + \sum_{i \in \mathcal{A}} \sum_{\ell \not\in \mathcal{A}} \varepsilon^{\mu \alpha \nu} V_{i \ell}^{\alpha \lambda} \langle \sigma_\ell^{\lambda} \sigma_i^{\nu} \prod_{j \in \mathcal{A} \setminus \{i\}} \sigma_j^{\mu_j} \rangle \tag{4.7}
\]

in which we see the characteristic form of a coupled hierarchy of differential equations: the time derivative of the correlator is given in terms of correlators between spins in \( \mathcal{A} \) and correlators among all possible subsets of \( \mathcal{A} \) with one spins removed, as well as all possible sets made from adding one spin to \( \mathcal{A} \). The local field term mixes up the different correlators between qubits in the cluster of qubits \( \mathcal{A} \), while the interaction terms “transfers correlations” to clusters which contain either one less or one more qubit.

The result (4.7) is still rather forbidding, mainly because it describes the dynamics of correlators for all of the spins contained in \( \mathcal{A} \). To make it more transparent, we now consider two special cases of this general result.

### 4.2.1 One- and Two-qubit Correlators

To simplify equation (4.7), we can make the subset \( \mathcal{A} \) small. We consider the two simplest cases, where \( \mathcal{A} \) includes one or two sites.

**Single-site \( \mathcal{A} \):** Suppose \( \mathcal{A} \) is just a single qubit - without loss of generality we call this “site 1”. Then there is only one correlator, given by the expectation value
\[ \langle \sigma_{1}^{\mu}(t) \rangle \); the equation of motion, read off from (4.7), is just

\[
\frac{d}{dt} \langle \sigma_{1}^{\mu} \rangle = \varepsilon^{\mu \alpha \beta} \left( h_{1}^{\alpha} \langle \sigma_{1}^{\beta} \rangle + \sum_{\ell \neq 1} V_{\ell}^{\alpha \lambda} \langle \sigma_{\ell}^{\lambda} \sigma_{1}^{\beta} \rangle \right)
\]  

(4.8)

where we recall that \( V_{ii}^{\alpha \beta} = 0 \), i.e., there is no on-site interaction apart from the local field \( h_{i} \), and we note again that the product over an empty set just gives unity for the 3rd term in (4.7). In vector notation eq. (4.8) reads

\[
\frac{d}{dt} \langle \sigma_{1} \rangle = (h_{1} + \tilde{V}_{1}) \times \langle \sigma_{1} \rangle
\]

(4.9)

where the total field \( \tilde{V}_{1} \) acting on \( \sigma_{1} \) from all the other qubits, via the interaction, has components

\[
\tilde{V}_{1}^{\alpha} = \sum_{\ell \neq 1} V_{\ell}^{\alpha \lambda} \langle \sigma_{\ell}^{\lambda} \rangle
\]

(4.10)

Thus (4.9) is simply telling us that spin 1 is precessing in a total field coming from the local external field plus the field on site 1 generated by all the other spins, via the interaction.

This result is of course well known, and can be derived trivially starting directly from the Hamiltonian. The second term in (4.9) can be thought of as a “Hartree” mean field interaction term.

**Two-site \( \mathcal{A} \):** Slightly less trivial is the result we get when \( \mathcal{A} \) incorporates a pair of sites, which we call site 1 and site 2. We are then interested in the dynamics of the pair correlator \( \langle \sigma_{1}^{\mu_{1}} \sigma_{2}^{\mu_{2}} \rangle \), and we find

\[
\frac{d}{dt} \langle \sigma_{1}^{\mu_{1}} \sigma_{2}^{\mu_{2}} \rangle = \sum_{j \neq j'} \varepsilon^{\mu_{j} \alpha \beta} \left[ h_{j}^{\alpha} \langle \sigma_{j}^{\beta} \sigma_{2}^{\mu_{j'}} \rangle + V_{12}^{\alpha \mu_{j'}} \langle \sigma_{j}^{\beta} \rangle \right] + \sum_{\ell \neq 1,2} V_{\ell}^{\alpha \lambda} \langle \sigma_{\ell}^{\lambda} \sigma_{j}^{\beta} \sigma_{j'}^{\mu_{j'}} \rangle
\]

(4.11)

where \( \sum_{j \neq j'} \) means that we sum over both \( j \) and \( j' \), with the restriction that \( j \neq j' \). This result contain both the fields we already saw for the single-site correlator (but now acting on both spins) plus a term - the 2nd term on the RHS in (4.11) above - which accounts for the interaction between the two spins.

We can now see intuitively how the results will develop as one goes to correlators including larger numbers of spins in \( \mathcal{A} \). It is also interesting to see how things simplify if we look at a very small total system. Thus, eg., suppose system \( \mathcal{S} \) comprises only \( N = 2 \) spins. Then the sub-system \( \mathcal{A} \) is just the whole system, and we expect the result to be trivial. Writing out all terms explicitly, we have

\[
\frac{d}{dt} \langle \sigma_{1}^{\mu_{1}} \sigma_{2}^{\mu_{2}} \rangle = \varepsilon^{\mu_{1} \alpha \beta} \left( h_{1}^{\alpha} \langle \sigma_{1}^{\beta} \sigma_{2}^{\mu_{2}} \rangle + V_{0}^{\alpha \mu_{2}} \langle \sigma_{1}^{\beta} \rangle \right) + \varepsilon^{\mu_{2} \alpha \beta} \left( h_{2}^{\alpha} \langle \sigma_{2}^{\beta} \sigma_{1}^{\mu_{1}} \rangle + V_{0}^{\alpha \mu_{1}} \langle \sigma_{2}^{\beta} \rangle \right)
\]

(4.12)
where we have written $V_{12} = V_0$ for the interspin interaction; the role of the effective fields acting on the one- and two-spin correlators is now transparent.

### 4.2.3 Relationship to Schwinger-Dyson Hierarchy

The Schwinger-Dyson hierarchy \[29, 69, 94, 95\] exists in both relativistic and non-relativistic forms - it is an infinite chain of coupled equations of motion for $n$-point correlators, whose specific form depends on the interactions in the theory being treated. Its general form is similar to the classical Bogoliubov Born Green Kirkwood Yvon (BBGKY) hierarchy.

To see how this related to what we have done, consider the Schwinger-Dyson hierarchy for a simple scalar field Lagrangian of form

$$L = \frac{1}{2} \phi \hat{K}_0^{-1} \phi - V(\phi)$$  \hspace{1cm} (4.13)

where $\hat{K}_0$ is the free field propagator. Here $x$ is a spacetime coordinate; and to be definite let us assume a simple local “pairwise” interaction, of form

$$V(\phi) = \frac{g}{4!} \phi^4(x)$$  \hspace{1cm} (4.14)

Then the Schwinger-Dyson hierarchy for the $n$-point correlation functions $G_n(\{x_j\})$, with $j = 1, \ldots, n$, is given by

$$K_0^{-1}(x,x)G_n(x,x_1', \ldots, x_{n-1}') - \frac{g}{6} G_{n+2}(x,x,x_1', \ldots, x_{n-1}') = i\hbar \sum_{j=1}^{n-1} \delta(x - x_j') \tilde{G}_{n-2}(\{x_j'\})$$  \hspace{1cm} (4.15)

where $K_0^{-1}(x,x') = \langle x | \hat{K}_0^{-1} | x' \rangle$. If we multiply (4.15) through by $\hat{K}_0$, we have

$$G_n(x,x_1', \ldots, x_{n-1}') + \frac{g}{6} \int d^4 z K_0(x-z) G_{n+2}(zzz,x_1', \ldots, x_{n-1}')$$

$$+ i\hbar \sum_{j=1}^{n-1} K_0(x-x_j') \tilde{G}_{n-2}(\{x_j'\}) = 0$$  \hspace{1cm} (4.16)

In both of these equations we define the “reduced” correlator $\tilde{G}_{n-2}(\{x_j'\})$ by

$$\tilde{G}_{n-2}(\{x_j\}) = G_{n-1}(x_1', \ldots, x_{j-1}', x_{j+1}', \ldots, x_{n-1}')$$  \hspace{1cm} (4.17)

from which the external legs with coordinates $x_j'$ and $x_n'$ have been removed.

The hierarchical form of equation (4.16), in which correlators $G_n$ are coupled to both higher and lower correlators, is very clear. Physically, one describes this equation by saying that if we have an excitation propagating from $x_j'$ to $x$ in the
presence of a set of mutually interacting excitations propagating between the points $x'_1, \cdots x'_j, \cdots x'_{j+1}, \cdots, x'_{n-1}$, then it can do so with or without interacting with the other excitations.

Mathematically, we see that the main differences between the Schwinger-Dyson hierarchy and the one we have derived here are:

(i) Here we are not dealing with the propagation of correlators like $G_n$ between different spacetime intervals, but instead with time-local correlators in which space does not appear (in its place we have cell or site indices $i, j, \cdots$).

(ii) In contrast with field theory where equations simplify because the variables are indistinguishable, the variables considered here on different cells or sites are distinguishable, and each such variable has to be identified explicitly in the equations of motion. This makes the equations more complex.

One can of course integrate equations like (4.3), (4.5), or (4.7), over time - in analogy with the passage from (4.15) to (4.16). The resulting form can be seen by choosing simple examples, such as the spin examples in (4.9) or (4.11). The same interpretation applies - the spins in $A$ can evolve with or without interacting with other spins outside $A$.

Such an approach is very useful when dealing with regular lattices of, eg., spins; then we can apply decoupling techniques to the resulting hierarchy very similar to those used for the Schwinger-Dyson equations.

However, in dealing with the general case, we would like to develop other approaches, to which we now turn.

4.3 Entanglement Correlators

Although the hierarchy of equations governing the dynamics of the different density matrices has a clear physical interpretation, and allows us to formulate the idea of different levels of entanglement, the equations of motion in the form given are not all that convenient to solve.

In what follows we set up a more useful description. The basic idea is fairly simple - we define a “supervector” whose components are an ordered list of all the different time-dependent correlation functions. We then derive a linear first-order differential equation for the time dependence of this vector.

To more easily explain the development, we do things first for a simple 2-spin problem, and then discuss some aspects of a general formulation of this kind - in particular, we describe how one treats a pair of coupled systems, and how to treat the equation of motion perturbatively, when there is a small parameter.
4.3.1 Example: Dynamics of a Single Qubit

For a single qubit \( \tau \) the most general Hamiltonian (upto an arbitrary constant term) is,

\[
H = \frac{1}{2} h \cdot \tau, \tag{4.18}
\]

here \( h \) is an effective applied field acting on the qubit. The equations of motion for the polarisation vector \( \langle \tau(t) \rangle \) are,

\[
\frac{d}{dt} \langle \tau(t) \rangle = h \times \langle \tau(t) \rangle = \begin{pmatrix}
0 & -h_z & h_y \\
h_z & 0 & -h_x \\
-h_y & h_x & 0
\end{pmatrix} \langle \tau(t) \rangle. \tag{4.19}
\]

The solution to the equation of motion can then be written conveniently in terms of the Green function for the equation of motion \( g(t) \),

\[
\langle \tau(t) \rangle = g(t) \langle \tau(0) \rangle. \tag{4.20}
\]

\( g(t) \) can be evaluated by taking the Laplace transform of the equation of motion (4.19)

\[
g(z) = \left[ zI - \begin{pmatrix}
0 & -h_z & h_y \\
h_z & 0 & -h_x \\
-h_y & h_x & 0
\end{pmatrix} \right]^{-1}, \tag{4.21}
\]

where \( I \) is the 3 \times 3 identity matrix. Which leads to the explicit formula for \( g(z) \)

\[
g^{\mu\nu}(z) = \frac{\hat{h}^\mu \hat{h}^\nu}{z} + \frac{\delta^{\mu\nu} - \hat{h}^\mu \hat{h}^\nu + i\varepsilon^{\mu\gamma\nu} \hat{h}_\gamma}{2(z - ih)} + \frac{\delta^{\mu\nu} - \hat{h}^\mu \hat{h}^\nu - i\varepsilon^{\mu\gamma\nu} \hat{h}_\gamma}{2(z + ih)}, \tag{4.22}
\]

where we have written the vector \( h \) in terms of its magnitude \( h \) and direction \( \hat{h} \). Inverting the Laplace transform then leads to

\[
g^{\mu\nu}(t) = \Theta(t) \hat{h}^\mu \hat{h}^\nu + \frac{e^{ht}}{2} \left( \delta^{\mu\nu} - \hat{h}^\mu \hat{h}^\nu + i\varepsilon^{\mu\gamma\nu} \hat{h}_\gamma \right) + \frac{e^{-ht}}{2} \left( \delta^{\mu\nu} - \hat{h}^\mu \hat{h}^\nu - i\varepsilon^{\mu\gamma\nu} \hat{h}_\gamma \right), \tag{4.23}
\]

\[
= \Theta(t) \left\{ \hat{h}^\mu \hat{h}^\nu + \cos(ht) \left( \delta^{\mu\nu} - \hat{h}^\mu \hat{h}^\nu \right) + \sin(ht) \varepsilon^{\mu\nu\lambda} \hat{h}_\lambda \right\}. \tag{4.24}
\]

Here \( \Theta(t) \) is the Heaviside step function. Equation (4.24) shows that \( g(t) \) is a matrix describing the rotation around the axis of the applied field, \( \hat{h} \) by an angle of \( ht \).

4.3.2 Example: Entanglement Correlator Dynamics: Two Qubits

For an arbitrary quantum system, the set of all possible observables is usually rather complicated. However in the case of spin systems, one can make an exhaustive list. For a single spin \( \tau \), the spin dynamics is completely defined by giving, as a function of time, the expectation values of all 3 components \( \langle \tau_\mu(t) \rangle \). For a pair of spins \( \tau_1 \)
and $\tau_2$, 15 different correlators are required, viz., $\langle \tau_1(t) \rangle$, $\langle \tau_2(t) \rangle$, and $\langle \tau_1 \otimes \tau_2 \rangle$, where this last contains components $\langle \tau_1^\mu(t) \tau_2^\nu(t) \rangle$. For a set of $N$ qubits, we need $2^{2N} - 1$ correlators.

To see how the general idea works, we go back to the example of two qubits, with Hamiltonian

$$H = \sum_{a=1}^{2} \frac{1}{2} h_a \cdot \tau_a + \frac{1}{2} V_{\mu\nu} \tau_1^\mu \tau_2^\nu$$

(4.25)

in which the orientation of the 2 static fields $h_1, h_2$ is arbitrary. This is just the Hamiltonian (4.6), for a pair of spins.

Now, suppose we arrange all the information contained in the 2-qubit density matrix (compare equation (3.10)) in the form of a 15-component “supervector” $X$ in the “space of possible correlators”, according to

$$X = \begin{pmatrix} X_1 \\ X_2 \\ X_3 \\ X_5 \\ X_6 \\ X_7 \\ X_8 \\ \vdots \end{pmatrix} = \begin{pmatrix} \langle \tau_1^x \rangle \\ \langle \tau_1^y \rangle \\ \langle \tau_1^z \rangle \\ \langle \tau_2^x \rangle \\ \langle \tau_2^y \rangle \\ \langle \tau_2^z \rangle \\ \langle \tau_1 \tau_2 \rangle \\ \vdots \end{pmatrix} \equiv \begin{pmatrix} \langle \tau_1 \rangle \\ \langle \tau_2 \rangle \\ \langle \tau_1 \otimes \tau_2 \rangle \end{pmatrix}.$$ 

(4.26)

We can then rewrite the hierarchy of equations of motion for the 2-qubit density matrix in the form

$$\frac{d}{dt} X = M X$$

(4.27)

or, written out explicitly, in the block structure

$$\frac{d}{dt} \begin{pmatrix} \langle \tau_1 \rangle \\ \langle \tau_2 \rangle \\ \langle \tau_1 \otimes \tau_2 \rangle \end{pmatrix} = \begin{pmatrix} L_1 & 0 & U_{1,p} \\ 0 & L_2 & U_{2,p} \\ U_{p,1} & U_{p,2} & L_p \end{pmatrix} \begin{pmatrix} \langle \tau_1 \rangle \\ \langle \tau_2 \rangle \\ \langle \tau_1 \otimes \tau_2 \rangle \end{pmatrix}.$$ 

(4.28)

Looking first at the diagonal matrix elements of $M$, we see that $L_1, L_2$ are $3 \times 3$ matrices which give an infinitesimal rotation of $\langle \tau_1 \rangle, \langle \tau_2 \rangle$ around the applied fields. The $9 \times 9$ matrix $L_p$ rotates the pair correlator $\langle \tau_1 \tau_2 \rangle$ around the applied fields, and can also be written as a rank 4 tensor (the lowered indices in the following expressions are understood to be contracted to the right in equation (4.28)). Thus we have:

$$L_1^{\mu\nu} = h_1^\lambda e^{\mu\lambda}_\nu$$

(4.29)

$$L_2^{\alpha\beta} = h_2^\gamma e^{\alpha\gamma}_\beta$$

(4.30)

$$L_p^{\mu\nu\alpha\beta} = L_1^{\mu\nu} \delta^\alpha_\beta + \delta^\mu_\nu L_2^{\alpha\beta}$$

(4.31)
Turning now to the non-diagonal interaction matrices, we have terms $U_{1,p}, U_{2,p}$ which are $3 \times 9$ matrices, and which create single qubit coherences from the pair correlator; the corresponding terms $U_{p,1}, U_{p,2}$ are $9 \times 3$ matrices which create pair coherences from the single qubit coherences. All of these interaction matrices may be represented as rank 3 tensors:

$$U_{1,p}^\mu_{\nu\beta} = V_{\lambda\beta}^{e \mu\lambda\nu}$$

$$U_{p,1}^\mu_{\alpha\nu} = V_{\lambda\nu}^{e \mu\lambda\alpha}$$

$$U_{2,p}^\alpha_{\nu\beta} = V_{\nu\gamma}^{e \alpha\gamma\beta}$$

$$U_{p,2}^\mu_{\alpha\beta} = V_{\mu\gamma}^{e \alpha\gamma\beta}.$$  

We see that the matrix $M\bar{M}$ is fully anti-symmetric and has eigenvalues which are either zero or pure imaginary. One can divide these into two classes, as follows:

(i) there are at least 3 zero eigenvectors of $M\bar{M}$, which are linear combinations of the eigenstates $|n\rangle\langle n|$ of the Hamiltonian (the dimensionality of the system of equations is one less than the number of components of the density matrix, because the equations automatically preserve the trace of the density matrix).

(ii) The other eigenvalues of $M\bar{M}$ occur at every difference $E_n - E_m$ in the eigenvalues of the Hamiltonian and their eigenvectors are off-diagonal elements of the density matrix $|n\rangle\langle m|$.

In general we can define a set of Green functions $\{g_{ij}\}$ with $i, j \in \{1, 2, p\}$ for the solution to the equations of motion (4.28), so that the solution to the equations of motion for the vector $X$ can be written

$$X(t) = G(t)X(0)$$

where the total propagator has the block form

$$G(t) = \begin{pmatrix} g_{11}(t) & g_{12}(t) & g_{1p}(t) \\ g_{21}(t) & g_{22}(t) & g_{2p}(t) \\ g_{p1}(t) & g_{p2}(t) & g_{pp}(t) \end{pmatrix}$$

A formal solution for this Green function is found by Laplace transforming; writing $f(z) = \int_0^\infty dt f(t)e^{-zt}$, we have

$$G(z) = [z\mathbb{I} - M]^{-1}.$$ 

so that $G(z)$ has poles at along the imaginary axis at all the differences between the energy eigenvalues $\pm i\Delta E$ as well as a pole at zero with a degeneracy of at least four.

In the time domain the Green function is just

$$G(t) = \exp(Mt) = \sum_{n=0}^{\infty} \frac{M^n t^n}{n!}.$$ 

(4.32)

(4.33)

(4.34)

(4.35)

(4.36)

(4.37)

(4.38)

(4.39)
This series can be represented graphically (see Fig. 4.2). We define a graph whose vertices are the possible correlators, having (directed) links between them which represent the block components of $M$. Then we an $n$-th order term in the sum is represented by a “walk” (i.e., sequence of $n$ hops) across $n$ links between nodes; multiplying each term by $t^n/n!$ we get the Green function.

It is important to get an idea of what these expressions look like in practice. Suppose we look first at a very simple case, where the Hamiltonian is

$$H = \frac{1}{2} [\Delta_1 \tau^x + \Delta_2 \sigma^x + \omega \tau^z \sigma^z]$$

having energy eigenvalues $\pm \epsilon_1, \pm \epsilon_2$ with

$$\epsilon_1 = \frac{1}{2} \sqrt{\omega^2 + (\Delta_1 + \Delta_2)^2}$$

$$\epsilon_2 = \frac{1}{2} \sqrt{\omega^2 + (\Delta_1 - \Delta_2)^2}.$$
eigenvalues of $M$ for this case are

$$\omega_{10} = (\epsilon_1 - \epsilon_2)$$  \hspace{1cm} (4.43)
$$\omega_{20} = \epsilon_1 + \epsilon_2$$  \hspace{1cm} (4.44)
$$\omega_{30} = 2\epsilon_1$$  \hspace{1cm} (4.45)
$$\omega_{21} = 2\epsilon_2.$$  \hspace{1cm} (4.46)

The different components of $G(t)$, i.e., the 9 different matrix Green functions given in equation (4.37) are then multiperiodic functions containing these 4 frequencies. Their explicit expressions are of course quite lengthy to write out; in App. C the explicit results for $G(z)$ are written in full.

The general 2-qubit Hamiltonian (4.25) is not much more complicated than this. In particular, the matrix $M$ has the key property that it is rather sparse, i.e., most elements are still zero. To see this, we write the interaction tensor in diagonal form, i.e., $V_{\mu\alpha} = V_{xx} \hat{x}_\mu \hat{x}_\alpha + V_{yy} \hat{y}_\mu \hat{y}_\alpha + V_{zz} \hat{z}_\mu \hat{z}_\alpha$; note that there is always a co-ordinate system where $V_{\mu\alpha}$ is of this form, which can be obtained using the singular value decomposition of $V_{\mu\alpha}$. Then the sub-matrices which make up $M$ can be written
explicitly as

\[
L_1 = \begin{pmatrix}
0 & -h \hat{z} & h \hat{y} \\
- h \hat{y} & h & 0 \\
- h \hat{y} & h \hat{z} & 0
\end{pmatrix}
\]  \hspace{1cm} (4.47)

\[
L_2 = \begin{pmatrix}
0 & -h \hat{z} & h \hat{y} \\
- h \hat{y} & h & 0 \\
- h \hat{y} & h \hat{z} & 0
\end{pmatrix}
\]  \hspace{1cm} (4.48)

\[
L_p = \begin{pmatrix}
0 & -h \hat{z} & h \hat{y} & -h \hat{z} & 0 & 0 & h \hat{y} & 0 & 0 \\
- h \hat{y} & h \hat{x} & 0 & 0 & 0 & -h \hat{z} & 0 & 0 & h \hat{y} \\
- h \hat{y} & h \hat{x} & 0 & 0 & 0 & -h \hat{z} & 0 & 0 & h \hat{y} \\
0 & h \hat{y} & 0 & 0 & h \hat{x} & 0 & h \hat{z} & 0 & -h \hat{y} \\
0 & 0 & -h \hat{y} & 0 & 0 & h \hat{x} & 0 & h \hat{z} & 0
\end{pmatrix}
\]  \hspace{1cm} (4.49)

\[
U_{1p} = \begin{pmatrix}
0 & 0 & 0 & 0 & 0 & -V_{zz} & 0 & V_{yy} & 0 \\
0 & 0 & V_{zz} & 0 & 0 & 0 & V_{yy} & 0 & 0 \\
0 & -V_{yy} & 0 & V_{xx} & 0 & 0 & 0 & 0 & 0
\end{pmatrix}
\]  \hspace{1cm} (4.50)

\[
U_{2p} = \begin{pmatrix}
0 & 0 & 0 & 0 & V_{yy} & 0 & -V_{zz} & 0 & 0 \\
0 & 0 & -V_{xx} & 0 & 0 & 0 & V_{zz} & 0 & 0 \\
0 & V_{xx} & 0 & -V_{yy} & 0 & 0 & 0 & 0 & 0
\end{pmatrix}
\]  \hspace{1cm} (4.51)

\[
U_{p1} = - U_{1p}^T \\
U_{p2} = - U_{2p}^T.
\]  \hspace{1cm} (4.52)

By making \( h_a = \hat{x} \Delta a \), and using a purely longitudinal coupling, we get back the simpler Hamiltonian in (4.40). In any case, we see that most elements in these matrices are zeroes.

More generally, so long as there are only local fields and pairwise interactions, it is evident that the “sparseness” of the matrix \( M \) will increase rapidly with the number of qubits.

### 4.4 Remarks on a General Formulation

Let us now consider how this might go for more complicated systems. The generalization of the 2-spin results to \( N \) spins is clear - now the supervector \( X \) has \( d_N = 2^N - 1 \) entries, growing very rapidly with \( N \).

More generally one may have to deal with systems in the thermodynamic limit, having an infinite number of degrees of freedom. Moreover, most degrees of freedom in Nature are usually described by continuous variables, and this automatically leads...
to an infinite set of possible correlators (such as the set $\langle x \rangle, \langle x, x' \rangle, \langle x, x', x'' \rangle, \cdots$, etc, for a single coordinate degree of freedom); and as noted in the introduction, the system may be composed of indistinguishable particles.

We will not deal with all these complications here - but it is still useful to understand some more general features of problems involving distinguishable spins. In what follows we look at two key questions, viz., (i) how do things work when we have 2 coupled spin systems, and (ii) if there is a small parameter in the problem, how do we make perturbation expansions for the entanglement correlators?

### 4.4.1 Two Coupled Systems

The special case of two separate but coupled systems is of interest for several reasons. Most notably, it forms the basis for a discussion of a central system coupled to some environment; and it is also useful when one comes to analyze how entanglement develops between any pair of systems.

Consider a pair of systems $S_1$ and $S_2$, which may or may not interact, and which are in general entangled. We again define an abstract supervector $\xi$ which contains all possible correlators for the pair of systems, in the form

$$\xi = \begin{pmatrix} X_1 \\ Y \\ X_2 \end{pmatrix}$$  \hspace{1cm} (4.54)

where $X_1$ is the vector containing all the correlators of operators acting on $S_1$ alone, $X_2$ likewise for $S_2$, and $Y$ refers to all “joint” operators, acting on both systems together.

As an example one can consider a pair of qubit systems, one containing $n_1$ spins $\{\tau_i\}$, and the other $n_2$ spin-$1/2$ degrees of freedom $\{\sigma_j\}$, with the total number of spins being $N = n_1 + n_2$. We then have

$$X_1 = \begin{pmatrix} \langle \tau_1^\alpha \rangle \\ \langle \tau_2^\alpha \rangle \\ \vdots \\ \langle \tau_1^\alpha \tau_2^\beta \rangle \\ \langle \tau_1^\alpha \tau_3^\beta \rangle \\ \vdots \\ \langle \tau_1^\alpha \tau_2^\beta \tau_3^\gamma \rangle \\ \vdots \end{pmatrix} \hspace{1cm} ; \hspace{1cm} X_2 = \begin{pmatrix} \langle \sigma_1^\alpha \rangle \\ \langle \sigma_2^\alpha \rangle \\ \vdots \\ \langle \sigma_1^\alpha \sigma_2^\beta \rangle \\ \langle \sigma_1^\alpha \sigma_3^\beta \rangle \\ \vdots \\ \langle \sigma_1^\alpha \sigma_2^\beta \sigma_3^\gamma \rangle \\ \vdots \end{pmatrix}$$  \hspace{1cm} (4.55)

for the supervectors of $S_1$ and $S_2$ respectively; the supervector $Y$ on the other hand
has the entries

\[ Y = \begin{pmatrix} \langle \tau_1^\mu \sigma_1^\alpha \rangle \\ \langle \tau_1^\mu \sigma_2^\alpha \rangle \\ \vdots \\ \langle \tau_2^\mu \sigma_1^\alpha \rangle \\ \langle \tau_2^\mu \sigma_2^\alpha \rangle \\ \vdots \\ \langle \tau_1^\mu \tau_2^\nu \sigma_1^\alpha \rangle \\ \vdots \\ \langle \tau_1^\mu \sigma_1^\alpha \sigma_2^\beta \rangle \\ \vdots \end{pmatrix} \]  

(4.56)

The number of components of these different vectors are then given by

\[ d_{X_1} = 2^{2n_1} - 1 \quad d_{X_2} = 2^{2n_2} - 1 \]

\[ dy = (2^{2n_1} - 1)(2^{2n_2} - 1) \]

\[ d_{X_1 + X_2} = d_N = 2^{2N} - 1 \]  

(4.57)

where \( N = (n_1 + n_2) \).

Let us now take the Laplace transform of \( \xi(t) \), defined as before by

\[ \xi(z) = \int_0^\infty dt e^{-zt} \xi(t) \]  

(4.58)

The equations of motion can then be written in the following form

\[ \xi(z) = \mathbb{G}(z) \xi(0) \]  

(4.59)

where \( \xi(0) \) is the initial value of \( \xi \) and \( \mathbb{G}(z) \) is a matrix, whose inverse has the following block structure:

\[ \mathbb{G}(z)^{-1} = \begin{pmatrix} g_1^{-1}(z) & -V_1M & 0 \\ -V_{M1} & g_M^{-1}(z) - V_{MM} & -V_{M2} \\ 0 & -V_{2M} & g_2^{-1}(z) \end{pmatrix} \]  

(4.60)

where the “mixed” propagator \( g_M \) in the middle matrix element \( M_{M,M} \) is given by

\[ g_M^{-1}(z) = g_1^{-1}(z)I_2 + g_2^{-1}(z)I_1 - zI_1I_2 \]  

(4.61)

In these equations \( X_j(z) = g_j(z)X(0) \) is the solution to the equations of motion for the individual system \( j \) (with \( j = 1, 2 \)) in the absence of any coupling between them; \( I_j \) is the identity acting on system \( j \), and the interaction matrix \( V \) has the form, in the same \( d_N \)-dimensional space,

\[ V = \begin{pmatrix} 0 & V_{1M} & 0 \\ V_{M1} & V_{MM} & V_{M2} \\ 0 & V_{2M} & 0 \end{pmatrix} \]  

(4.62)
The elements of the sub matrices of \( V \) can be obtained as needed by reading them off from the equations of motion (for which of course we require a specific Hamiltonian).

In general the \( G(z) \) will have poles at \( z = i(\omega_n - \omega_m) \) for all \( n, m \) where \( \omega_n \) is the \( n \)th energy eigenvalue of the Hamiltonian. The pole at \( z = 0 \) will be of at least of order \( 2^{n_1-n_2} - 1 \), with larger orders occurring when the system has degenerate energy levels.

When the systems are large it does not make sense to be enumerating all the poles and their residues. Instead we simply define a spectral function which gives us the density of the poles along the imaginary axis; we write

\[
\kappa(\omega) = \frac{1}{2\pi} [G(i\omega + \epsilon) - G(i\omega - \epsilon)]
\] (4.63)

where we choose \( \epsilon \) to be small but still larger than the typical separation between poles. For sufficiently large systems the poles will become so close that we can treat them as defining a branch cut along the imaginary axis, with magnitude \( \kappa(\omega) \).

### 4.4.2 Perturbation Expansions

Suppose we have solved the full hierarchy in some specific case, and we add a small term to the Hamiltonian, - this could be, eg., to each of the bath spin local fields, or to the interaction between the central systems and the bath spins. The question is how a perturbation theory will be structured.

We do not give a full treatment here, since it is rather messy. The simplest case is the one in which we treat the interaction term \( V \) as a perturbation. We can then write an equation for the full Green function, \( G(z) \) as an expansion about the \( V = 0 \) Green function, \( G_0(z) \), where in this case one has

\[
G_0(z) \equiv \left( \begin{array}{ccc}
g_1(z) & 0 & 0 \\
0 & g_M(z) & 0 \\
0 & 0 & g_2(z)
\end{array} \right). \quad (4.64)
\]

A Dyson series for \( G(z) \) may then be obtained in through the usual manipulations,

\[
G(z) = [G_0^{-1}(z) - V]^{-1}
\] (4.65)

\[
= G_0(z) \sum_{n=0}^{\infty} (VG_0(z))^n \quad (4.66)
\]

where the matrix being raised to the \( n \)-th power is just

\[
VG_0(z) = \left( \begin{array}{ccc}
0 & V_{1M}g_M(z) & 0 \\
V_{M1}g_1(z) & V_{MM}g_M(z) & V_{M2}g_2(z) \\
0 & V_{2M}g_M(z) & 0
\end{array} \right) \quad (4.67)
\]

Note that care needs to be taken when this expansion is performed near the high order poles of \( G_0(z) \), to ensure that the corrections are still small.
4.5 Conclusion

We have used the entanglement correlated part of the reduced density matrix to derive a hierarchy of equations of motion linking the motion for reduced density matrices. This hierarchy links the reduced density matrix \( \hat{\rho}_A \) on a subset of the system \( A \) to reduced density matrices on all sets obtained by adding one cell to \( A \).

Then we derived a linear hierarchy of equations for systems of qubits, linking different orders of correlators. We found that the time of a derivative correlator containing pauli matrices acting on a cluster \( A \) of qubits, depends on correlators on clusters obtained by adding or removing one qubit from \( A \). Then we presented results for a single qubit and a pair of qubits, and saw how the equations could be solved for Green functions which propagate different correlators.

The structure of the hierarchy of equations for spin correlators was then investigated in more detail. In particular we saw how the evolution of correlators in a system consisting of two distinct sets of qubits. We discuss this case in more detail in the next chapter, with the case in mind where one of the sets of qubits is the environment. We will formally “integrate out” this set of environmental qubits and examine the structure of the resulting solution for the central qubits’ motion.

Then in following chapters, the hierarchy of equations for qubit correlators will be used, to gain an understanding of the process by which central qubits lose information into correlations with the environment.
Chapter 5

Integrating a Spin Bath Out of the Hierarchy

In this chapter we consider the effect a set $B$ of “environmental spins” on the remaining system spins. We use the structure of the hierarchy of equations of motion for qubit correlators described in chapter 4 when there is an environmental spin bath present. We eliminate the bath spins and derive formal expressions for the Green functions describing the evolution of correlators between system qubits only. The result is a formal expression for the dynamics of the system correlators, which gives us insight into how the bath spins can affect the motion of the central spins. Then we consider the special case where the environment and the bath are initially in a product state.

We consider $N_S$ “central” $\frac{1}{2}$–spins \{\(\tau_a\) \((a = 1, \ldots, N_S)\) coupled to $N_B$ bath spins \{\(\sigma_i\) \((i = 1, 2, \ldots, N_B)\). In general the full density matrix $\rho$ can be written,

$$
\rho = \frac{1}{2^{N_A+N_B}} \left\{ 1 + \sum_{a=1}^{N_S} \langle \tau_a^\mu \rangle \tau_a^\mu + \sum_{i=1}^{N_B} \langle \sigma_i^\alpha \rangle \sigma_i^\alpha + \langle \tau_1^\mu \tau_2^\nu \rangle \tau_1^\mu \tau_2^\nu + \sum_{i=1}^{N_B} \sum_{a=1}^{N_S} \langle \tau_a^\mu \sigma_i^\alpha \rangle \tau_a^\mu \sigma_i^\alpha + \sum_{i=1}^{N_B} \sum_{j<i} \langle \sigma_j^\beta \sigma_i^\alpha \rangle \sigma_j^\beta \sigma_i^\alpha + \ldots \right\} \quad (5.1)
$$

in the above and in what follows, $i, j, k \ldots \in \{1, 2, \ldots, N_B\}$ index bath spins and $a, b, c \ldots \in \{1, 2\}$ index central spins. In the above the terms “…” involve sums over all distinct clusters of spin operators. All information about the system at a given time (including the bath) is contained in the density matrix. We can construct a super vector $\xi(t)$ of these correlators just like in section 4.4.1 where in this case system one is the central system $S$ and system two is the bath $B$.

Assume the Hamiltonian is of the following form,

$$
H = \frac{1}{2} \sum_{a=1}^{N_S} \mathbf{h}_a \cdot \tau_a + \frac{1}{2} \sum_{a=1}^{N_S} \sum_{b<a} u_{ab}^\mu \tau_a^\mu \tau_b^\nu + \frac{1}{2} \sum_{a=1}^{N_S} \sum_{i=1}^{N_B} V_{a\mu}^i \tau_a^\mu \sigma_i^\alpha + \frac{1}{2} \sum_{i=1}^{N_B} \mathbf{b}_i \cdot \sigma_i. \quad (5.2)
$$

For completeness we give the hierarchy of equations of motion in this case. Let $C$ be a subset of the central system containing $m$ spins (the form written here will be valid for a central system containing an arbitrary number of spins) and $A$ be
a subset of the bath containing \( n \) spins the equation of motion for the equal time correlator \( \langle \prod_{a \in C} \tau_a^{i \mu} \prod_{i \in A} \sigma_i^{a i} \rangle \) is,

\[
\begin{aligned}
\frac{d}{dt} \langle \prod_{a \in C} \tau_a^{i \mu} \prod_{i \in A} \sigma_i^{a i} \rangle &= \sum_{a \in C} \varepsilon_{a \mu \nu} \langle \tau_a^{i \nu} \prod_{b \in C \setminus \{a\}} \tau_b^{c \mu} \prod_{i \in A} \sigma_i^{a i} \rangle \\
&+ \sum_{b \in C \setminus \{a\}} u_{b \mu b} \langle \tau_a^{i \nu} \prod_{c \in A \setminus \{a, b\}} \sigma_i^{c i} \rangle + \sum_{b \in S \setminus C} u_{b \gamma b} \langle \tau_a^{i \nu} \tau_c^{c \gamma} \prod_{i \in A} \sigma_i^{a i} \rangle \\
&+ \sum_{j \in A} V_{aj}^{\nu \alpha} \langle \sigma_j^{\beta} \prod_{a \in C \setminus \{a\}} \tau_a^{i \mu} \prod_{i \in A \setminus \{j\}} \sigma_i^{a i} \rangle + \sum_{b \in B \setminus A} V_{bj}^{\nu \beta} \langle \sigma_j^{\beta} \prod_{a \in C \setminus \{b\}} \tau_a^{i \mu} \prod_{i \in A \setminus \{j\}} \sigma_i^{a i} \rangle \\
&+ \sum_{b \in S \setminus A} V_{b \kappa}^{\nu \beta} \langle \sigma_j^{\beta} \prod_{a \in C} \tau_a^{i \mu} \prod_{i \in A \setminus \{j\}} \sigma_i^{a i} \rangle.
\end{aligned}
\] (5.3)

The various terms in equation (5.3) are illustrated in figure 5.1.

The equation of motion (5.3) is of the form

\[
\frac{d\xi}{dt} = M\xi,
\] (5.4)

when written in terms of the supervector of correlators. After we take the Laplace transform of \( \xi(t) \), we find that the equation of motion may indeed be written in the form of equation (4.59), which we repeat here for clarity,

\[
\xi(z) = G(z)\xi(0).
\] (5.5)

Where \( \xi(0) \) is the initial value of \( \xi \) and \( G(z) \) is a matrix, whose inverse has the following block structure:

\[
G(z)^{-1} = \begin{pmatrix}
g_{S}^{-1}(z) & -V_{S,M} & 0 \\
-V_{M,S} & g_{M}^{-1}(z) - V_{M,M} & -V_{M,B} \\
0 & -V_{B,M} & g_{B}^{-1}(z)
\end{pmatrix}
\] (5.6)

and \( g_{M}^{-1} \) is as in equation (4.61). Note that \( G(z)^{-1} \) is of the form

\[
G(z)^{-1} = zI - M.
\] (5.7)

Also in this case \( g_{S} \) and \( g_{B} \) are \((2^{NS} - 1) \times (2^{NS} - 1)\) and \((2^{2NS} - 1) \times (2^{2NS} - 1)\) matrices respectively. All the terms \( V_{AC} (A, C \in \{S, M, B\}) \) are due to the interaction \( V_{\mu a} \) between the system and the bath. The matrix elements relating to the various \( V \) submatricies in can be read off the equations of motion. For example,
Figure 5.1: The various terms appearing in equation (5.3) when there are three central qubits and three bath spins. Right, an illustration of a possible choices of the set $\mathcal{A}$ in red, which contains some central qubits (represented by green dots) and some bath qubits (represented by blue dots). The left hand figure shows the terms on the right hand side of equation (5.3). Terms are in the same order in the equation as in the figure. In each term, a correlator between qubits in the shaded set, the local field acting on circled qubits, and the interaction $u(V)$ acting between qubits linked by green (dark red) dashed lines enter into the corresponding term in equation (5.3). Note the second, fourth, and seventh terms on the right hand side of equation (5.3) are each represented by two diagrams in the figure, as each of these terms has a sum over two correlators.
$V_{MM}$ acts on mixed correlators $\left\langle \prod_{a \in C} \tau_a^{\mu_a} \prod_{j \in A} \sigma_j^{\alpha_j} \right\rangle$ and produces correlators which have one less or one more spin. So there are some matrix elements in $V_{MM}$ which give a contribution to the time derivative of the correlator with one of the bath spins (say $i$) removed
\[
\frac{d}{dt} \left\langle \prod_{a \in C} \tau_a^{\mu_a} \prod_{j \in A \setminus \{i\}} \sigma_j^{\alpha_j} \right\rangle,
\]
this contribution is
\[
\sum_{c \in C} \varepsilon^{\mu_c \lambda_c} V_{ci}^{\nu_c} \left\langle \tau_c^{\nu_c} \sigma_i^{\lambda_c} \prod_{a \in C} \tau_a^{\mu_a} \prod_{j \in A \setminus \{i\}} \sigma_j^{\alpha_j} \right\rangle. \tag{5.8}
\]

### 5.1 Integrating Out the Bath Spins

The bath spins can be formally integrated out by inverting the matrix $G(z) = zI - M$, there are multiple ways to do this, in what follows we describe two.

In the first approach one inverts $(zI - M)$ by performing elementary row reduction to reduce $(zI - M)$ to an upper triangular matrix, then complete the process of row reduction to invert the matrix. When the $(zI - M)$ is inverted in this manner this the top “block-row” (which is what is needed to obtain $X(z)$ the correlators specifying the state of the central system in terms of all of the initial correlators) of $(zI - M)^{-1}$ can be written,

\[
G_{SS}(z) = g_S V_{SM} \tilde{G}_{MM} \left[ I_M - V_{MB} G_{BB} V_{MB}^T \right]^{-1} \tilde{G}_{MM} V_{SM} g_S, \tag{5.9}
\]

\[
G_{SM}(z) = g_S V_{SM} \tilde{G}_{MM} \left[ I_M - V_{MB} G_{BB} V_{MB}^T \tilde{G}_{MM} \right] \tag{5.10}
\]

\[
G_{SB}(z) = g_S V_{SM} \tilde{G}_{MM} V_{MB} G_{BB}. \tag{5.11}
\]

with

\[
\tilde{G}_{MM} = [(g_M)^{-1} - V_{MM} - V_{SM} g_S V_{SM}]^{-1} \tag{5.12}
\]

\[
G_{BB} = [(g_S)^{-1} - V_{MB}^T \tilde{G}_{MM} V_{MB}]^{-1}. \tag{5.13}
\]

Note that $G_{BB}$ is an exact sub-matrix of $G(z)$. Also note that in the above we could define the $\{G_{SS}, G_{SM}, \ldots\}$ as the Laplace transforms of the following quantities,

\[
G_{AC}(t) = \frac{\partial \xi_A(t)}{\partial \xi_C(0)} \bigg|_{\xi(0)=0} \quad A, C \in \{S, M, B\}. \tag{5.14}
\]

Where we have defined the super vectors $\xi_S \equiv X_S$, $\xi_B \equiv X_B$, and $\xi_M \equiv Y$.

We can interpret the results (5.9–5.13) as follows. $\tilde{G}_{MM}$ in equation (5.12) is the Green function which gives a contributions to mixed correlators from mixed correlators. The “self energy” term $V_{SM}^T g_S V_{SM}$ includes all the terms where mixed
correlators evolve into system only correlators then back into mixed correlators (so \( \tilde{G}_{MM} \) includes the back-reaction terms from \( X_S \)). \( \tilde{G}_{MM} \) can then be used to calculate the exact bath-bath Green function (5.13), because bath correlators are only sourced by mixed correlators or by bath correlators. The last term in (5.13) can be seen as the effect of all the mixed and system correlators on the dynamics on bath only correlators. Once one has the exact bath-bath Green function one can get the exact the exact bath-system Green function (5.11) by including the propagation of correlations through the mixed correlators to the central system. One can also then calculate the mixed Green function (5.10) using \( \tilde{G}_{MM} \) to propagate mixed correlators from to system correlators including the possibility that the mixed correlators back-react through the bath correlators (the second term in equation (5.10) is the self energy for this effect). Then the full system-system Green function (5.9) is given by the “bare” system system Green function corrected by the possibilities of backreaction; through the set of mixed correlators and through the set of bath correlators via the mixed correlators (the second to last and last term respectively in equation (5.9)).

In the second approach inverts \((zI-M)\) by performing elementary row reduction to reduce \((zI-M)\) to an lower triangular matrix as a first step, after the inversion is complete one gets,

\[
G_{SM} = G_{SS}V_{SM}G_2 
\]

(5.15)

\[
G_{SB} = G_{SM}V_{MB}g_B 
\]

(5.16)

with

\[
G_2 = \left[(g_M)^{-1} - V_{MB}g_BV_{MB}^T\right]^{-1} 
\]

(5.17)

\[
G_{SS} = \left[(g_S)^{-1} - V_{SM}G_2V_{SM}^T\right]^{-1} 
\]

(5.18)

The representation of the inverse in equations (5.15-5.18) is in a sense the opposite to that (5.9-5.13). The effective mixed-mixed Green function including back-reaction only through the bath correlators is calculated first in equation (5.17) (instead of including only back-reaction through system correlators in the previous approach). From which one can immediately calculate the exact system-system Green function (5.18) by including back-reaction through the mixed correlators. It is then no trouble to get the mixed-system (5.15) and bath-system (5.16) Green functions.

The different sets of formulae (5.15-5.18) and (5.9-5.13) for the Green functions are of course only two of many such formulae.

Now we discuss the structure of the different Green functions in the complex plane. As discussed in section 4.3.2 \( G(z) \) has poles along the imaginary axis, at points determined by the differences between eigenvalues of the Hamiltonian (5.2). In general this means all the sub matrices of \( G(z) \) have poles at these frequencies, though the weights of these poles may be very different. For instance the Green functions \( G_{SB} \) and \( G_{SM} \) are zero when there is no interaction between the bath and central system.
5.1.1 Product State Initial Conditions

Often we will be interested in the case where initially the system is in a product state $\rho(0) = \rho_S(0) \otimes \rho_B(0)$ this implies that initially we will be able to write $Y(0) = X_S(0) \otimes X_B(0) \equiv X_0^S \otimes X_0^B$. In this case the solution for the vector $X_S$ which contains all the information about the central system can be written:

$$X_S(z) = \left[ G_{SS} + G_{SM} X_0^B \otimes \right] X_0^S + G_{SB} X_S$$(5.19)

$$\equiv G_{X_S}(z, \{\sigma_k^0\}) X_0^S + J_S(z, \{\sigma_k^0\})$$(5.20)

So we can see that the correlators in the central system are propagated by a propagator which is renormalised by the effect of the bath and the correlations in the bath can also generate correlations in the central system. We can write a definition for $G_{X_S}(z, \{\sigma_k^0\}), J_S(z, \{\sigma_k^0\})$ as follows

$$G_{X_S}(z, \{\sigma_k^0\}) \equiv \frac{\partial X_S(t)}{\partial X_B(0)} \bigg|_{\xi(0) = (X_S(0), X_S(0) \otimes X_B(0), 0)^T}$$ (5.22)

$$J_S(z, \{\sigma_k^0\}) \equiv \frac{\partial X_S(t)}{\partial X_B(0)} \bigg|_{\xi(0) = (0, 0, X_B(0))^T}$$ (5.23)

5.2 Conclusion

We have seen that when studying the dynamics of a qubit system coupled to a spin bath the set of correlators can divided into system, mixed, and bath correlators. We can integrate out the bath spins and find effective dynamics for the central system correlators, including terms that are sourced by the mixed and bath correlators.

We have also seen how the Green functions for the correlators inherit their singularities from the inverses of the dynamical matrix and how that depends on fixed block structure of that matrix. Finally we have simplified the results for case with product state initial conditions and we see the propagation off the system correlators still in general depends on a “source” term in which the initial conditions on the bath can source system correlators.

In following chapters we will turn to more practical applications and examples where we can use the hierarchy of equations to model the interaction of central qubits coupled to an environment.
Chapter 6

Overview of Simple Single Qubit Models

Now we consider some simple single central qubit models and discuss their dynamics. Most of the work in this chapter is an original take on models and results previously studied in the literature. We also derive some new results for these models.

The first model we consider is the of a central qubit coupled to a spin bath in the degeneracy blocking regime introduced in section [1.7.2] we develop a picture for the loss of information by the central system into correlators with the environment. Then we discuss a central qubit under the influence of a time varying field caused by an external source. We then treat a case when this time varying force is stochastic and can be averaged (we discuss performing the bias average introduced in section [1.7.2]).

6.1 Example, Degeneracy Blocking Spin Bath

Consider a central spin $\tau$ coupled to a spin bath consisting of N spins $\{\sigma_i\}$ with the Hamiltonian $[19, 86, 88]$,

$$
H = \frac{\Delta_0^2}{2} \tau^x + \sum_{j=1}^{N} \frac{1}{2} \omega_j \tau^z \sigma_j^z.
$$

(6.1)

So we have a central qubit which may flip with an amplitude $\Delta_0$ and the states have an energy difference set by their coupling to bath spin variables. The bath spin variables cannot flip with respect to the $z$ axis. Prokof’ev and Stamp named the mechanism of the central qubits decay this model “degeneracy blocking”, because in states with $\sum_{j=1}^{N} \frac{1}{2} \omega_j \sigma_j^z \gg \Delta_0$” the central spin is blocked from flipping by the lack of degeneracy with the state they would flip into. As $\sigma_j^z$ commutes with the Hamiltonian this is simple to solve.

Define the bath states $|\eta\rangle = \prod_{j=1}^{N} |\eta_j\rangle$ specified by a length $N$ vector $\eta = (\eta_1, \eta_2, \ldots, \eta_N)$, whose entries, $\eta_i = \pm 1$ specify the orientation of the bath spins with respect to the $z$ axis. In terms of this basis the Hamiltonian is

$$
H = \sum_{\eta} \left( \frac{\Delta_0}{2} \tau^x + \sum_{j=1}^{N} \frac{1}{2} \omega_j \eta_j \tau^z \right) |\eta\rangle \langle \eta|.
$$

(6.2)
Thus the Hamiltonian can be viewed as a sum over different system Hamiltonians for each bath state. We can define $h_\eta$ to be the effective "magnetic field” acting on a qubit when the bath is in the state $|\eta\rangle$,

$$h_\eta \equiv \Delta_0 \hat{x} + \sum_j \omega_j \eta_j \hat{z}.$$  \hspace{1cm} (6.3)

The energy eigenvalues associated with a specific bath configuration $|\eta\rangle$ are,

$$\pm h_\eta = \pm \frac{1}{2} \sqrt{\Delta_0^2 + \left( \sum_{j=1}^N \frac{1}{2} \omega_j \eta_j \right)^2}.$$ \hspace{1cm} (6.4)

So that the evolution operator $U(t)$ can be written in the same form as the Hamiltonian (6.2),

$$U(t) = \sum_\eta e^{-\frac{i}{2}h_\eta \cdot \tau t} |\eta\rangle \langle \eta|.$$ \hspace{1cm} (6.5)

Therefore if the total density matrix is initially $\rho(0)$, then the density matrix after time $t$ is then

$$\rho(t) = \sum_\eta \sum_{\tilde{\eta}} |\eta\rangle e^{-\frac{i}{2}h_\eta \cdot \tau t} \langle \eta| \rho(0) |\tilde{\eta}\rangle e^{\frac{i}{2}h_{\tilde{\eta}} \cdot \tau t} \langle \tilde{\eta}|.$$ \hspace{1cm} (6.6)

Tracing out the bath, one then obtains the exact reduced density matrix $\bar{\rho}_S(t)$ for the central system,

$$\bar{\rho}_S(t) = \sum_\eta e^{-\frac{i}{2}h_\eta \cdot \tau t} \langle \eta| \rho(0) |\eta\rangle e^{\frac{i}{2}h_\eta \cdot \tau t}.$$ \hspace{1cm} (6.7)

So the reduced density matrix for the central system is the sum over contributions from each of the possible configurations of the bath spins. In each of these contributions effective magnetic field on the central is determined by the configuration of the bath spins. The operator $\langle \eta| \rho(0) |\eta\rangle$ (which acts on the system Hilbert space only) appearing in the expression (6.7) can be written in terms of correlators,

$$\langle \eta| \rho(0) |\eta\rangle = \frac{1}{2^{N+1}} \sum_{S\subseteq B} \left( \prod_{j\in C} \sigma_j^z \right) + \tau \cdot \left( \prod_{j\in C} \sigma_j^z \right) \prod_j \eta_j.$$ \hspace{1cm} (6.8)

Note that the expression for the system’s reduced density matrix (6.7) is true regardless of the initial state. In particular it still holds if the central spin is initially entangled with the bath. However if the system is initially separable from the bath $\rho(0) = \bar{\rho}_S(0)\bar{\rho}_B(0)$ then the solution (6.7) simplifies to an average over an ensemble of static biases,

$$\bar{\rho}_S(t) = \int_{-\infty}^{\infty} d\xi \ P_{DB}(\xi) \ e^{-\frac{i}{2}h(\xi) \cdot \tau t} \bar{\rho}_S(0) e^{\frac{i}{2}h(\xi) \cdot \tau t},$$ \hspace{1cm} (6.9)
where \( h(\xi) \equiv \Delta_0 \hat{x} + \xi \hat{z} \) when the bias is \( \xi \) and \( P_{DB}(\xi) \) is the distribution of biases. The distribution of biases is set by the baths initial state,

\[
P_{DB}(\xi) \equiv \sum_\eta \delta \left( \xi - \sum_j \omega_j \eta_j \right) \langle \eta | \hat{\rho}_B(0) | \eta \rangle.
\] (6.10)

The delta functions in equation (6.10) can be summed to give an almost continuous bias distribution if either: the bath state represents an ensemble of a large number of states or if there are a large number of bath spins and the bath is initially in a (potentially pure) state with out a definite bias, \( \hat{\xi} = \sum_i \omega_i \sigma_i^z \). The decay of different elements of the density matrix in this model is caused by interference of components with different biases. Note that distribution of biases (6.10) only depends on the diagonal parts of the bath density matrix. So that for instance the system evolution will be the same whether the bath is prepared in the pure state

\[
\hat{\rho}_B(0) = \prod_j (| \uparrow \rangle_j \langle \uparrow |_j + | \downarrow \rangle_j \langle \downarrow |_j)
\] (6.11)

or if the bath is prepared in the impure state

\[
\hat{\rho}_B(0) = \frac{1}{2^N} I.
\] (6.12)

The polarisation \( \langle \tau(t) \rangle \) of the central spin is also averaged in the same way as the central spin reduced density matrix,

\[
\langle \tau(t) \rangle = \int_{-\infty}^{\infty} d\xi \ P_{DB}(\xi) \ g(t; \xi) \cdot \langle \tau(0) \rangle.
\] (6.13)

Here \( g(t; \xi) \) is the single qubit Green function from equation (4.24) with the field \( h = h(\xi) \).

### 6.1.1 Example: Gaussian Bias Distribution

Here we consider the specific case of a Gaussian bias distribution with standard deviation \( \delta \xi \) centred around \( \xi = 0 \), that is

\[
P_{DB}(\xi) = \frac{e^{-\xi^2/(2\delta^2\xi^2)}}{\sqrt{2\pi}\delta \xi}.
\] (6.14)

This distribution naturally arises from the law of large numbers when many uncorrelated random factors contribute to the bias. For example if the bath is initially prepared in either of the states (6.11) or (6.11), all the couplings \( \omega_i = \omega_0 \) are the same, there are a large number \( N \) of bath spins, and the coupling is small enough. Then the distribution of biases will be approximately that given by equation (6.14)
with $\delta \xi = \frac{1}{4} \sqrt{N} \omega_0$. The Green function is the averaged of the Green functions for each bias,

$$g^{\mu\nu}(t) \equiv \int_{-\infty}^{\infty} d\xi \, P_{DB}(\xi) \, g^{\mu\nu}(t; \xi)$$

$$= \Theta(t) \int_{-\infty}^{\infty} d\xi \, P_{DB}(\xi) \, \hat{h}^\mu(\xi) \hat{h}^\nu(\xi)$$

$$+ \text{Re} \int_{-\infty}^{\infty} d\xi \, P_{DB}(\xi) \, e^{i\hat{h}(\xi)t} (\delta^{\mu\nu} - \hat{h}(\xi) \hat{h}(\xi)_{\mu}^\nu + i\varepsilon^{\mu\nu\gamma} \hat{h}_{\gamma}(\xi)) \, (6.15)$$

$$= \Theta(t) \int_{-\infty}^{\infty} d\xi \, P_{DB}(\xi) \, e^{i\hat{h}(\xi)t} (\delta^{\mu\nu} - \hat{h}(\xi) \hat{h}(\xi)_{\mu}^\nu + i\varepsilon^{\mu\nu\gamma} \hat{h}_{\gamma}(\xi)) \, \hat{h}^\mu(\xi) \hat{h}^\nu(\xi)$$

$$+ \text{Re} \int_{-\infty}^{\infty} d\xi \, P_{DB}(\xi) \, e^{i\hat{h}(\xi)t} (\delta^{\mu\nu} - \hat{h}(\xi) \hat{h}(\xi)_{\mu}^\nu + i\varepsilon^{\mu\nu\gamma} \hat{h}_{\gamma}(\xi)) \, (6.16)$$

Using the symmetry of the bias distribution we have

$$g^{\mu\nu}(t) = \Theta(t) \int_{-\frac{\Delta_0}{\Delta}}^{\frac{\Delta_0}{\Delta}} d\omega A(\omega) \left[ \hat{z}^\mu \hat{z}^\nu + \frac{\Delta_0^2}{\omega} (\hat{x}^\mu \hat{x}^\nu - \hat{z}^\mu \hat{z}^\nu) \right]$$

$$+ \text{Re} \int_{-\frac{\Delta_0}{\Delta}}^{\frac{\Delta_0}{\Delta}} d\omega A(\omega) e^{i\omega t} \left[ \delta^{\mu\nu} - \hat{z}^\mu \hat{z}^\nu + \frac{\Delta_0^2}{\omega} (\hat{x}^\mu \hat{x}^\nu - \hat{z}^\mu \hat{z}^\nu) \right]$$

$$+ i \frac{\Delta_0}{\omega} \varepsilon^{\mu1\nu}$$

$$\text{(6.17)}$$

with $A(\omega) = \sqrt{\frac{2}{\pi \delta \xi}} e^{-\omega^2 \Delta_0^2} \sqrt{\frac{1}{1 - \left(\frac{\Delta_0}{\omega}\right)^2}}$.

$\text{(6.18)}$

So the pole that we had before in the Laplace transform of the single qubit Green function is smeared out into a branch cut and long time behavior of (6.18) is determined by the singularity at the branch point $\omega = \Delta_0$. At long times $g^{\mu\nu}(t)$ will oscillate around $g^{\mu\nu}_{\infty}$,

$$g^{\mu\nu}_{\infty} = \int_{-\frac{\Delta_0}{\Delta}}^{\frac{\Delta_0}{\Delta}} d\omega A(\omega) \left[ \hat{z}^\mu \hat{z}^\nu + \frac{\Delta_0^2}{\omega} (\hat{x}^\mu \hat{x}^\nu - \hat{z}^\mu \hat{z}^\nu) \right]$$

$$= \hat{z}^\mu \hat{z}^\nu + \sqrt{\frac{\pi \Delta_0}{2 \delta \xi}} e^{\frac{\Delta_0^2}{2 \delta \xi}} \text{erfc} \left( \frac{\Delta_0}{\sqrt{2 \delta \xi}} \right) \left[ \hat{x}^\mu \hat{x}^\nu - \hat{z}^\mu \hat{z}^\nu \right].$$

$\text{(6.19)}$

Where erfc denotes a complementary error function [26]. The long time oscillations will have a frequency $\Delta_0$ and the different components to the oscillation amplitudes will die down like,

$$g^{\mu\nu}(t) \sim g^{\mu\nu}_{\infty} + \text{Re} \left\{ \frac{e^{i\Delta t - i\frac{\pi}{4}}}{\Delta \pi \delta \xi \sqrt{2t}} \left( \hat{z}^\mu \hat{z}^\nu + \hat{y}^\mu \hat{y}^\nu + i\varepsilon^{\mu1\nu} + \frac{3}{4\Delta^2 \delta^2} \hat{x}^\mu \hat{x}^\nu \right) \right\}$$

$\text{(6.20)}$

as $t \rightarrow +\infty$ (in this expression I have kept the leading order term for each independent tensor component). Examining the long time solution we see we only get coherent rotation of the central qubit polarisation vector around the $x$ axis and that the components of the polarisation vector in the $z - y$ plane die down slower than those in the $x$ direction. This is because averaging over both positive and negative biases means that all rotation of components around the $z$ axis due to the bias field is averaged out.
6.1.2 Return Probability

Of particular interest to us is the probability $p_r(t)$ that the central spin will return to its initial state after a given time, this can be calculated in our formalism. Let $C$ stand for the central system and $B$ stand for the bath then if the central system starts in a state $|\psi\rangle$ unentangled with the bath state $|\Phi_B\rangle$ so that the total wave function $|\Psi(0)\rangle = |\psi\rangle \otimes |\Phi_B\rangle$ then the return probability is

$$ p_r = \text{tr}_B \left( \langle \psi \right| U(t) |\Psi\rangle \langle U^\dagger(t) |\psi\rangle \right) $$

(6.22)

$$ = \text{tr}_C \left( |\psi\rangle \langle \psi | \bar{\rho}_C(t) \right) $$

(6.23)

$$ = \frac{1}{4} \text{tr} \left[ (I + \langle \tau(0) \rangle \cdot \tau)(I + \langle \tau(t) \rangle \cdot \tau) \right] $$

(6.24)

$$ = \frac{1}{2} (1 + \langle \tau(0) \rangle \cdot \langle \tau(t) \rangle) $$

(6.25)

$$ = \frac{1}{2} \left( 1 + \langle \tau^\mu(0) \rangle \langle \tau^\nu(0) \rangle g^{\mu\nu}(t) \right). $$

(6.26)

So the symmetric part of $g^{\mu\nu}(t)$ determines the return probability in one qubit systems and in the case of degeneracy blocking for long times we have

$$ p_r(t) \sim \frac{1}{2} \left\{ 1 + \langle \tau^x(0) \rangle^2 \left( g^{xx}_\infty + \frac{3 \cos \left( \Delta t - \frac{\pi}{4} \right)}{4\sqrt{2} \pi \delta \xi \Delta_0^3 t^{5/2}} \right) \right. $$

(6.27)

$$ + \langle \tau^y(0) \rangle^2 \left( g^{yy}_\infty + \frac{\cos \left( \Delta_0 t - \frac{\pi}{4} \right)}{\Delta_0 \pi \delta \xi \sqrt{2} t} \right) $$

$$ + \langle \tau^z(0) \rangle^2 \left( g^{zz}_\infty + \frac{\cos \left( \Delta_0 t - \frac{\pi}{4} \right)}{\Delta_0 \pi \delta \xi \sqrt{2} t} \right) \right\}. $$

6.1.3 Decay of the Central Qubit Polarisation

In this model the polarisation of the central qubit (and therefore the purity of its density matrix) decays. Indeed for generic separable initial conditions for the total density matrix $\rho(0) = \frac{1}{2} (1 + \langle \tau(0) \rangle \cdot \tau) \bar{\rho}_B(0)$, in the case discussed in the previous section where $\bar{\rho}_B(0)$ results in a Gaussian distribution for the bias, the long time central qubit polarisation,

$$ \langle \tau(t) \rangle^2 = (g_\infty \langle \tau(0) \rangle)^2 + O(t^{-1/2}). $$

(6.28)

So that the central qubit’s polarisation decays to an initial condition dependent constant, with the slowest decaying components decaying with $t^{-1/2}$.

The decay of the polarisation indicates that information is lost to the environmental bath. It is reasonable to ask, how does this information decay into the environment?
We can start by using the hierarchy of equations of motion (5.3) to derive an expression for the rate of change of the central qubit polarization

\[ \frac{d}{dt} \langle \tau \rangle^2 = 2 \sum_j \omega_j (\hat{z} \times \langle \tau \sigma^z_j \rangle) \cdot \langle \tau \rangle. \]  

(6.29)

Thus the decay of the central qubit polarization depends on the correlators \( \langle \tau x \sigma^z_j \rangle \) and \( \langle \tau x \sigma^z_j \rangle \). In fact in this model the only correlators involving bath spins which affect the dynamics of the central spin are of the form \( \langle \tau(t) \prod_{j \in C} \sigma^z_j(t) \rangle \) (for \( C \subseteq B \)). This is because there is a closed subset of the hierarchy of equations,

\[ \frac{d}{dt} \langle \tau(t) \prod_{j \in C} \sigma^z_j(t) \rangle = \Delta_0 \hat{z} \times \langle \tau(t) \prod_{j \in C} \sigma^z_j(t) \rangle \]  

(6.30)

\[ + \sum_{\ell \not\in C} \omega_\ell \hat{z} \times \langle \tau(t) \sigma^z_\ell(t) \prod_{j \in C} \sigma^z_j(t) \rangle \] 

\[ + \sum_{\ell \in C} \omega_\ell \hat{z} \times \langle \tau(t) \prod_{j \in C \setminus \{\ell\}} \sigma^z_j(t) \rangle, \]

which involve only these correlators. In fact we can calculate these correlators exactly,

\[ \langle \tau(t) \prod_{j \in C} \sigma^z_j(t) \rangle = \frac{1}{2^N} \sum_{n=0}^{N-|C|} \binom{N}{n} \binom{|C|}{m} (-1)^m g(t; -N\omega_0 + 2\omega_0(m + n)) \cdot \langle \tau(0) \rangle. \]  

(6.31)

In the case where there is an equal likelihood of any given initial bath spin configuration (that is \( \langle \eta | \tilde{\rho}(0) | \eta \rangle = \frac{1}{2^N} \)) and all bath spins have the same couplings \( \omega_j = \omega_0 \), then we have,

\[ \langle \tau(t) \prod_{j \in C} \sigma^z_j(t) \rangle = \frac{1}{2^N} \sum_{n=0}^{N-|C|} \binom{N-|C|}{n} \]  

\[ \cdot \sum_{m=0}^{|C|} \binom{|C|}{m} (-1)^m g(t; -N\omega_0 + 2\omega_0(m + n)) \cdot \langle \tau(0) \rangle. \]  

(6.32)

Before we discuss what these solutions actually look like, we note that correlators of the form (6.32) are the only non-zero correlators that arise in the evolution of the density matrix from the chosen initial conditions. Before we prove this statement, we note that it implies equation (6.32) actually gives us exact expressions for the connected correlators (whether we define these as the coefficients in the Pauli expansion of either \( \tilde{\rho}^C \) or \( \tilde{\rho}^{CC} \), discussed in chapter [2]). We now prove that the only
non-zero correlators are of the form $\langle \tau(t) \prod_{j \in C} \sigma_j^z(t) \rangle$, for some subset of the bath $C$. First note that any possible correlator can be written in the either of the forms,

$$\langle \tau^\mu \prod_{i \in A} \sigma_i^{a_i} \prod_{j \in C} \sigma_j^z \rangle \quad (6.33)$$

$$\langle \prod_{i \in A} \sigma_i^{a_i} \prod_{j \in C} \sigma_j^z \rangle \quad (6.34)$$

for appropriate choices of the disjoint bath subsets $A, C$ (which may be the zero set), the index $\mu$, and the indices $\{a_i\}$ which may take the values $a_i = 1 (x), 2 (y)$. Therefore the entire hierarchy of equations of motion can be written,

$$\frac{d}{dt} \langle \tau^\mu \prod_{i \in A} \sigma_i^{a_i} \prod_{j \in C} \sigma_j^z \rangle = \Delta_0 \epsilon^{\mu 1 \nu} \langle \tau^\nu \prod_{i \in A} \sigma_i^{a_i} \prod_{j \in C} \sigma_j^z \rangle \quad (6.35)$$

$$+ \sum_{\ell \in A} \omega_{\ell} \epsilon^{\mu 3 \ell} \langle \sigma_{\ell}^{\beta} \prod_{i \in A \setminus \{\ell\}} \sigma_i^{a_i} \prod_{j \in C} \sigma_j^z \rangle$$

$$+ \sum_{k \notin A \cup B} \omega_k \epsilon^{\mu 3 \nu} \langle \tau^\nu \prod_{i \in A} \sigma_i^{a_i} \prod_{j \in C \cup \{k\}} \sigma_j^z \rangle$$

$$+ \sum_{q \notin A} \omega_q \epsilon^{\mu 3 \nu} \langle \tau^\nu \prod_{i \in A} \sigma_i^{a_i} \prod_{j \in C \setminus \{q\}} \sigma_j^z \rangle.$$

$$\frac{d}{dt} \langle \prod_{i \in A} \sigma_i^{a_i} \prod_{j \in C} \sigma_j^z \rangle = \sum_{\ell \in A} \omega_{\ell} \epsilon^{\mu 3 \ell} \langle \tau^\nu \sigma_{\ell}^{\beta} \prod_{i \in A \setminus \{\ell\}} \sigma_i^{a_i} \prod_{j \in C} \sigma_j^z \rangle. \quad (6.36)$$

Notice that in equations (6.35) and (6.36), the only values of the index $\beta$ give non-zero contributions are $\beta = 1, 2$. This means that all correlators appearing on the right hand sides of equations (6.35) (6.36) contain off-diagonal bath Pauli matrices acting on qubits in the set $A$. So for a fixed set $A$, the set of equations (6.35) (6.36) with all applicable choices for the indices and set $C$, constitute a closed subset of the full hierarchy of equations of motion. Therefore for each $A \neq \emptyset$, there is a closed subset of linear equations of motion for the correlators of the form (6.33) (6.34) and because all these correlators are zero initially, the unique solution to this subset of equations is zero. When $A = \emptyset$ the equation (6.36) reduces to

$$\frac{d}{dt} \langle \prod_{j \in C} \sigma_j^z \rangle = 0,$$

and as these correlators are initially zero, they remain zero. We have now shown all the correlators except those of the form $\langle \tau^\mu \prod_{j \in C} \sigma_j^z \rangle$ are zero.
We have plotted increasing orders of correlators of this form with a range different values of the parameters \( \Delta_0, \omega_0 \), and \( N \) in figures 6.1-6.6. We have plots with 100 bath spins (figures 6.1, 6.3) and \( N = 10 \) (figures 6.4, 6.6) bath spins. We show systems where the standard deviation of the biases on the central spin are \( \frac{1}{2} \sqrt{N \omega_0} = \frac{1}{4} \Delta_0 \) (figures 6.1 and 6.4), \( \frac{1}{2} \sqrt{N \omega_0} = \Delta_0 \) (figures 6.2 and 6.5), and \( \frac{1}{2} \sqrt{N \omega_0} = 4 \Delta_0 \) (figures 6.3 and 6.6), one can think of these as systems with weak, intermediate, and strong coupling respectively. We focus on the initial decay behaviour of the solutions, at times before \( 2\pi/\omega_0 \), when there are approximate recurrences. What we see is, in all cases, as the central qubit’s polarisation decays there is a cascade of coherence. The coherence lost by the central qubit correlators is then is transferred to the second order correlators, then some portion of this is transferred to the third order correlators and so on. This process occurs rapidly, correlators containing seven bath spins are populated quickly. In the systems with larger baths and smaller couplings, correlators of all orders appear to tend toward a “steady state” value (until recurrences). Note that the order of magnitudes of different sized correlators can vary drastically. In particular it appears from the figures 6.1-6.6 that the more possible choices there are for correlators of a given order (e.g. are \( \binom{N}{2} \) third order correlators of the form \( \langle \tau^\mu \sigma^i_z \sigma^j_z \rangle \)) the smaller in magnitude correlators of that order will be. So it is desirable to consider a measure of the total strength of correlations of a given order, which is what we turn to now.

Recall from chapter one the purity of the full density matrix is \( p(t) = \text{tr} \rho^2(t) \) and as discussed in chapter 1 it gives a measure of how much information is contained in the full density matrix. The purity of the full density matrix is conserved (this is easy to show: \( \dot{p} = -i \text{tr}([H, \rho] \rho + \rho[H, \rho]) = 0 \)). We can therefor get an idea of how much information is stored in correlators of different orders by computing their contribution to the purity. Using the definition of the purity, the Pauli expansion of the density matrix (5.1), and our knowledge of the symmetry of the non-zero correlators in this case we have,

\[
p = \frac{1}{2^{N+1}} \left\{ 1 + \sum_{C \subseteq B} \left\langle \tau \prod_{i \in C} \sigma_i^z \right\rangle^2 \right\} \quad (6.38)
\]

\[
= \frac{1}{2^{N+1}} \left\{ 1 + \sum_{n=0}^{N} \binom{N}{n} \left\langle \tau \prod_{i=1}^{n} \sigma_i^z \right\rangle^2 \right\}. \quad (6.39)
\]

So we can define the part of the purity contained in the \( n \)--partite correlations \( c_n \) by,

\[
c_n \equiv \binom{N}{n-1} \left\langle \tau \prod_{i=1}^{n-1} \sigma_i^z \right\rangle^2, \quad (6.40)
\]

(we will call this the \( n \)-partite correlation strength). In figures 6.7-6.12 we have plotted the time dependence of \( c_n \)’s of different orders for the same cases described in
Figure 6.1: Plots of the correlators of the form $\langle \tau^\mu \prod_j \sigma^z_j \rangle$ for the degeneracy blocking model described in section 6.1.2. Values are computed from equation (6.32). In the case plotted there are $N = 100$ bath spins, their couplings are all $\omega_0 = \frac{1}{20} \Delta_0$ (so $\frac{1}{2} \sqrt{N}\omega_0 = \frac{1}{4} \Delta_0$), and the initial reduced density matrix for the system is $\bar{\rho}_S(0) = \frac{1}{2} (1 + \tau^x)$. In all figures the solid red curve is $\langle \tau^x \prod_j \sigma^z_j \rangle$, the dashed green curve is $\langle \tau^y \prod_j \sigma^z_j \rangle$, and the dotted blue curve is $\langle \tau^z \prod_j \sigma^z_j \rangle$. The left hand figure shows the first eight correlators and the right hand figure shows higher order correlators.
Figure 6.2: Plots of the correlators of the form $\langle \tau \prod_{j}^{n} \sigma_{j}^{z} \rangle$ for the degeneracy blocking model described in section 6.1.2. Values are computed from equation (6.32). In the case plotted there are $N = 100$ bath spins, their couplings are all $\omega_{0} = \frac{1}{2} \Delta_{0}$ (so $\frac{1}{2} \sqrt{N} \omega_{0} = \Delta_{0}$), and the initial reduced density matrix for the system is $\bar{\rho}_{S}(0) = \frac{1}{2} (1 + \tau^{x})$. In all figures the solid red curve is $\langle \tau \prod_{j}^{n} \sigma_{j}^{x} \rangle$, the dashed green curve is $\langle \tau \prod_{j}^{n} \sigma_{j}^{y} \rangle$, and the dotted blue curve is $\langle \tau \prod_{j}^{n} \sigma_{j}^{z} \rangle$. The left hand figure shows the first eight correlators and the right hand figure shows higher order correlators.
Figure 6.3: Plots of the correlators of the form $\langle \tau^\mu \prod_j \sigma_j^z \rangle$ for the degeneracy blocking model described in section 6.1.2. Values are computed from equation (6.32). In the case plotted there are $N = 100$ bath spins, their couplings are all $\omega_0 = \frac{4}{3} \Delta_0$ (so $\frac{1}{2} \sqrt{N} \omega_0 = 4 \Delta_0$), and the initial reduced density matrix for the system is $\bar{\rho}_S(0) = \frac{1}{2} (1 + \tau^x)$. In all figures the solid red curve is $\langle \tau^x \prod_j \sigma_j^z \rangle$, the dashed green curve is $\langle \tau^y \prod_j \sigma_j^z \rangle$, and the dotted blue curve is $\langle \tau^z \prod_j \sigma_j^z \rangle$. The left hand figure shows the first eight correlators and the right hand figure shows higher order correlators.
Figure 6.4: Plots of the correlators of the form $\langle \tau^\mu \prod_0^n \sigma_j^z \rangle$ for the degeneracy blocking model described in section 6.1.2. Values are computed from equation (6.32). In the case plotted there are $N = 10$ bath spins, their couplings are all $\omega_0 \approx 0.1581 \Delta_0$ ($\frac{1}{2} \sqrt{N} \omega_0 = \frac{1}{2} \Delta_0$), and the initial reduced density matrix for the system is $\tilde{\rho}_S(0) = \frac{1}{2} (1 + \tau^x)$. In all figures the solid red curve is $\langle \tau^x \prod_0^n \sigma_j^z \rangle$, the dashed green curve is $\langle \tau^y \prod_0^n \sigma_j^z \rangle$, and the dotted blue curve is $\langle \tau^z \prod_0^n \sigma_j^z \rangle$. 
Figure 6.5: Plots of the correlators of the form $\langle \tau^\mu \prod_j^n \sigma_j^z \rangle$ for the degeneracy blocking model described in section 6.1.2. Values are computed from equation (6.32). In the case plotted there are $N = 10$ bath spins, their couplings are all $\omega_0 \approx 0.6325 \Delta_0 \left( \frac{1}{2} \sqrt{N} \omega_0 = \Delta_0 \right)$, and the initial reduced density matrix for the system is $\bar{\rho}_S(0) = \frac{1}{2} (1 + \tau^x)$. In all figures the solid red curve is $\langle \tau^x \prod_j^n \sigma_j^z \rangle$, the dashed green curve is $\langle \tau^y \prod_j^n \sigma_j^z \rangle$, and the dotted blue curve is $\langle \tau^z \prod_j^n \sigma_j^z \rangle$. 
Figure 6.6: Plots of the correlators of the form $\langle \tau^\mu \prod_j^n \sigma_j^z \rangle$ for the degeneracy blocking model described in section 6.1.2. Values are computed from equation (6.32). In the case plotted there are $N = 10$ bath spins, their couplings are all $\omega_0 \approx 2.529 \Delta_0$ ($\frac{1}{2} \sqrt{N} \omega_0 = 4 \Delta_0$), and the initial reduced density matrix for the system is $\bar{\rho}_S(0) = \frac{1}{2} (1 + \tau^x)$. In all figures the solid red curve is $\langle \tau^x \prod_j^n \sigma_j^z \rangle$, the dashed green curve is $\langle \tau^y \prod_j^n \sigma_j^z \rangle$, and the dotted blue curve is $\langle \tau^z \prod_j^n \sigma_j^z \rangle$. 
Figure 6.7: The $n$–partite correlation strength for the degeneracy blocking model described in section 6.1.2. Values are computed from equation (6.32) and the definition for $c_n$ (6.40). In the case plotted there are $N = 100$ bath spins, their couplings are all $\omega_0 = \frac{1}{2\pi} \Delta_0$ (so $\sqrt[4]{N}\omega_0 = \frac{1}{4} \Delta_0$), and the initial reduced density matrix for the system is $\bar{\rho}_S(0) = \frac{1}{2} (1 + \tau_x)$.

the previous paragraph. From these figures we see that a portion of the correlation strength is cascaded between different orders. In the cases where we can see a definite “steady state” emerge (those with $N = 100$ and strong to intermediate coupling strength), the steady state $n$–partite correlation strength decreases with the order (at least for orders $n < N/2$).

Before we move on to other examples, an obvious question one can ask is, does the picture we have developed in this section of the decay central qubit’s polarisation as a cascade into higher order correlations hold in more complicated models that describe decoherence? We attempt to answer this for one model of decoherence in chapter 7.
Figure 6.8: The $n$–partite correlation strength for the degeneracy blocking model described in section 6.1.2. Values are computed from equation (6.32) and the definition for $c_n$ (6.40). In the case plotted there are $N = 100$ bath spins, their couplings are all $\omega_0 = \frac{1}{4} \Delta_0$ (so $\frac{1}{2} \sqrt{N} \omega_0 = \Delta_0$), and the initial reduced density matrix for the system is $\tilde{\rho}_S(0) = \frac{1}{2} (1 + \tau^x)$. 
Figure 6.9: The $n$-partite correlation strength for the degeneracy blocking model described in section 6.1.2. Values are computed from equation (6.32) and the definition for $c_n$ (6.40). In the case plotted there are $N = 100$ bath spins, their couplings are all $\omega_0 = \frac{1}{2} \Delta_0$ (so $\frac{1}{2} \sqrt{N} \omega_0 = 4 \Delta_0$), and the initial reduced density matrix for the system is $\tilde{\rho}_S(0) = \frac{1}{2} (1 + \tau^x)$. 
Figure 6.10: The $n$–partite correlation strength for the degeneracy blocking model described in section 6.1.2. Values are computed from equation (6.32) and the definition for $c_n$ (6.40). In the case plotted there are $N = 10$ bath spins, their couplings are all $\omega_0 \approx 0.1581\Delta_0$ ($\frac{1}{2}\sqrt{N}\omega_0 = \frac{1}{3}\Delta_0$), and the initial reduced density matrix for the system is $\bar{\rho}_S(0) = \frac{1}{2}(1 + \tau^x)$. 
Figure 6.11: The \( n \)-partite correlation strength for the degeneracy blocking model described in section 6.1.2. Values are computed from equation (6.32) and the definition for \( c_n \) (6.40). In the case plotted there are \( N = 10 \) bath spins, their couplings are all \( \omega_0 \approx 0.6325 \Delta_0 \left( \frac{1}{2} \sqrt{N \omega_0} = \Delta_0 \right) \), and the initial reduced density matrix for the system is \( \tilde{\rho}_S(0) = \frac{1}{2} (1 + \tau^x) \).
Figure 6.12: The $n$–partite correlation strenght for the degeneracy blocking model described in section 6.1.2. Values are computed from equation (6.32) and the definition for $c_n$ (6.40). In the case plotted there are $N = 10$ bath spins, their couplings are all $\omega_0 \approx 2.529\Delta_0$ ($\frac{1}{2}\sqrt{N}\omega_0 = 4\Delta_0$), and the initial reduced density matrix for the system is $\bar{\rho}_S(0) = \frac{1}{2}(1 + \tau^x)$. 
6.2 Example: Motion of Spin in Time Dependent Bias

In the previous section we studied a model where the effect of an external environment on the central spin is to average the energy bias on the central qubit. In this section we will consider the case where an external bias can result in a time dependent bias on the central system, which will prepare us to tackle the problem of averaging over a random dynamics bias in the next section. These kinds of models should be used with caution as the neglect quantum correlations built up between the central system and the environment. Consider the Hamiltonian describing a two level system with constant flipping probability and a time dependent bias

\[ H = \frac{1}{2} \Delta_0 \tau^x + \frac{1}{2} \xi(t) \tau^z. \]  

(6.41)

The equation of motion for \( \langle \tau(t) \rangle \) is,

\[ \frac{d}{dt} \langle \tau(t) \rangle = \left[ \Delta_0 \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} + \xi(t) \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \right] \langle \tau(t) \rangle. \]  

(6.42)

While this equation of motion is not exactly solvable we can write down a formal solution, which we now describe. Begin by solving the problem in the \( \Delta_0 = 0 \) case, this leads us to the Green function \( g_0 \),

\[ g_0(t, t') = \exp \left( -\int_{t'}^t ds \xi(s) \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \right) = \begin{pmatrix} \cos \theta(t, t') & \sin \theta(t, t') & 0 \\ -\sin \theta(t, t') & \cos \theta(t, t') & 0 \\ 0 & 0 & 1 \end{pmatrix} \]  

(6.43)

with \( \theta(t, t') = \int_{t'}^t ds \xi(s) \).

(6.44)

In the time between \( t' \) and \( t \) the zero \( \Delta_0 \) Green function rotates the qubits polarisation around the z axis by an angle \( \theta(t, t') \). The final total Green function \( g(t, t') \) is related to this by, the usual Dyson series

\[ \Delta = \Delta_0 \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} \]  

(6.45)

\[ g(t, t') = g_0(t, t') + \int_{t'}^t ds g_0(t, s) \Delta g(s, t') \]  

(6.46)

\[ = g_0(t, t') + \sum_{n=1}^{\infty} \left( \int_{t'}^t ds_n g_0(t, s_n) \Delta \right) \left( \int_{s_n}^{s_{n-1}} ds_{n-1} g_0(s_n, s_{n-1}) \Delta \right) \ldots \]  

\[ \left( \int_{t'}^{s_2} ds_1 g_0(s_2, s_1) \Delta \right) g_0(s_1, t'). \]  

(6.47)
This formal series solution is the best we can do without specifying more about the
time dependence of the bias field. We note that the series (6.47) solution to this
problem is equivalent to writing the Green function in terms of the time ordered
exponential \( \mathcal{T} \exp \)

\[
g(t, t') = \mathcal{T} \exp \left\{ \int_{t'}^t ds [\Delta + \xi(s)] \right\},
\]

with

\[
\xi(t) \equiv \xi(t) \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}.
\]

Numerical evaluation of these kind of formulae is discussed in appendix [D].

### 6.3 Randomly Fluctuating Force

We now consider models where the bias is fluctuating randomly over time. This
may be because the system is coupled to some fluctuating bath variable. In that
case the model is only applicable where the central systems dynamics do not effect
the bath dynamics in any appreciable way. We are talking about the case where the
Hamiltonian is (6.41) but where the functions \( \xi(t) \) are drawn from some probability
distribution described by a probability distribution functional \( P[\xi(t)] \). We denote
averages over this probability distribution by \( \langle \ldots \rangle_\xi \), the average of quantity \( Q[\xi] \) is
given by the functional integral (see for example [35]),

\[
\langle Q[\xi] \rangle_\xi \equiv \int \mathcal{D}\xi P[\xi] Q[\xi].
\]

Obviously there are many different specifications for the probability distribution
which are interesting, below we discuss one specific case.

#### 6.3.1 Gaussian Noise

Consider the case where \( \xi(t) \) has a Gaussian probability distribution function defined
by a correlator \( K(t, t') \):

\[
P[\xi] \equiv \mathcal{N} \exp \left\{ -\frac{1}{2} \int d\tau_1 \int d\tau_2 \xi(\tau_1) K^{-1}(\tau_1, \tau_2) \xi(\tau_2) \right\}
\]

\[
K(t, t') = \langle \xi(t) \xi(t') \rangle_\xi
\]

Then one can use the well known relationship [35],

\[
\langle e^{i \int_0^t ds \xi(s)} \rangle_\xi = \exp \left[ i \int_0^t ds_1 \langle \xi(s_1) \rangle_\xi - \int_0^t ds_1 \int_0^t ds_2 K(s_1, s_2) \right]
\]

to calculate the exact Green function in the absence of flipping. Now we work with
a specific form for noise correlator.
6.3.2 Example: Low frequency noise, diffusing bias

Now consider the case [86] where $\xi(t)$ is randomly fluctuating with

$$\langle |\xi(t) - \xi(t')|^2 \rangle_\xi = \Lambda^3 |t - t'|.$$  \hspace{1cm} (6.54)

That is the bias field under goes Brownian motion. Then the Green function in the absence of flipping averaged over the bias, $\langle g_0(t) \rangle_\xi$ is then

$$\langle g_0(t) \rangle_\xi = \begin{pmatrix} \cos(\xi_0 t)e^{-\Lambda^3|t|^3/6} & \sin(\xi_0 t)e^{-\Lambda^3|t|^3/6} & 0 \\ -\sin(\xi_0 t)e^{-\Lambda^3|t|^3/6} & \cos(\xi_0 t)e^{-\Lambda^3|t|^3/6} & 0 \\ 0 & 0 & 1 \end{pmatrix}. \hspace{1cm} (6.55)$$

Consider the regime where the diffusion is fast so that $\Lambda \gg |\Delta_0|$. The averaged solution to the equation of motion is shown in figure [6,13]. We see that the components of the polarisation in the $x - y$ plane decay more rapidly than the $z$ component, there is however some coherent oscillation between the $y$ and $z$ components.

We can understand this behaviour analytically. Components of the central qubit polarisation components $\langle \langle \tau^x \rangle \rangle_\xi$ and $\langle \langle \tau^y \rangle \rangle_\xi$, which are perpendicular to the diffusing field die down rapidly. To leading order we have

$$\begin{pmatrix} \langle \langle \tau^x \rangle \rangle_\xi \\ \langle \langle \tau^y \rangle \rangle_\xi \end{pmatrix} = \begin{pmatrix} \cos(\xi_0 t)e^{-\Lambda^3|t|^3/6} & \sin(\xi_0 t)e^{-\Lambda^3|t|^3/6} \\ -\sin(\xi_0 t)e^{-\Lambda^3|t|^3/6} & \cos(\xi_0 t)e^{-\Lambda^3|t|^3/6} \end{pmatrix} \begin{pmatrix} \sqrt{\xi_0} \mathbb{I} \\ \mathbb{I} \end{pmatrix} + \mathcal{O}(\Delta_0^2). \hspace{1cm} (6.56)$$

For the decay of $\langle \tau^z \rangle$ to occur the flipping term is necessary. We will now attempt to calculate the rate of this slower decay. We define an “interaction picture” polarisation vector $\langle \tau(t) \rangle_I$, which is the measured polarisation in a frame rotated according to the bias field alone,

$$\langle \tau(t) \rangle_I = g_0(0, t) \langle \tau(t) \rangle.$$

Then the equation of motion for $\langle \tau(t) \rangle_I$ is

$$\frac{d}{dt} \langle \tau(t) \rangle_I = g_0(0, t) \Delta g_0^T(0, t) \langle \tau(t) \rangle_I. \hspace{1cm} (6.58)$$

The formal solution to equation (6.58) is

$$\langle \tau(t) \rangle_I = \int_0^t dt_1 g_0(0, t_1) \Delta g_0^T(0, t_1) \langle \tau(t_1) \rangle_I + \langle \tau(0) \rangle. \hspace{1cm} (6.59)$$

Substituting the right hand side of equation (6.59) back into itself gives,

$$\langle \tau(t) \rangle = \int_0^t dt_2 g_0(t, t_2) \Delta \int_0^{t_2} dt_1 g_0(t_2, t_1) \langle \tau(t_1) \rangle$$

$$+ \int_0^t dt_1 g_0(t, t_1) \Delta g_0(t_1, 0) \langle \tau(0) \rangle + g(t_1, 0) \langle \tau(0) \rangle. \hspace{1cm} (6.60)$$
Figure 6.13: Plots of some solutions to the diffusing bias model discussed in section 6.3.2 calculated using the methods described in appendix D. In both cases the parameters are chosen so that $\Delta_0 = 0.1\Lambda$ and $\xi_0 = 0$. In both figures the solid red curve is $\langle\langle \tau^z(t) \rangle \rangle_\xi$, the dashed green curve is $\langle\langle \tau^y(t) \rangle \rangle_\xi$, and the dotted blue curve is $\langle\langle \tau^x(t) \rangle \rangle_\xi$ computed using the method described in appendix D.1. In the top figure the initial configuration of the central spin is $\langle \tau(0) \rangle = \hat{y}$ and the back curve is the $\Delta_0$ solution for $\langle\langle \tau^y(t) \rangle \rangle_\xi$ calculated using equation (6.56). In the bottom figure the initial configuration of the central spin is $\langle \tau(0) \rangle = \hat{z}$ and the back curve is the solution calculated using the integro-differential equation (6.63). The inset figure on the bottom shows the considerably smaller $\langle\langle \tau^x(t) \rangle \rangle_\xi$, and $\langle\langle \tau^y(t) \rangle \rangle_\xi$ components of the polarisation. The thin black curve in the inset plot shows the $y$ component of the polarisation computed numerically from the equation $\frac{d}{dt} \langle\langle \tau^z \rangle \rangle_\xi = \Delta_0 \langle\langle \tau^z \rangle \rangle_\xi$ and the numerical values of the $z$ component rather than the direct method in the appendix.
Differentiating and taking the z component gives

\[ \frac{d}{dt} \langle \tau(t) \rangle = \int_0^t ds_1 \Delta g_0(t, s_1) \Delta \langle \tau(s_1) \rangle \]  \hspace{1cm} (6.61)

\[ \frac{d}{dt} \langle \tau^z(t) \rangle = -\Delta^2 \int_0^t ds_1 \cos \left( \int_{s_1}^t ds_2 \xi(s_1) \right) \langle \tau^z(s_1) \rangle. \]  \hspace{1cm} (6.62)

Now take the average over the rapidly varying field \( \xi(t) \). Assuming that (6.62) can be written as an integral of a product of independent averages,

\[ \frac{d}{dt} \langle \langle \tau^z(t) \rangle \rangle_{\xi} = -\Delta^2 \int_0^t ds_1 \text{Re} \left( e^{i \xi_0(t-s_1) - \frac{1}{2} \Lambda^3 (t-s_1)^3} \right) \langle \langle \tau^z(s_1) \rangle \rangle_{\xi}. \]  \hspace{1cm} (6.63)

The integro-differential equation (6.63) can be solved numerically (we use the ID-SOLVER package [42] for MATLAB), this solution is compared against the full numerical solution to the motion in figure 6.13. We see that the integro-differential differential equation (6.63) is only accurate for short times. The reason for this is as follows. The central spin will only flip between its two z states when the bias is not much greater than the tunneling element \( \Delta_0 \) and because this element is small compared to the time scale for the diffusion of the bias field, this will only occur rarely when the bias diffuses to zero. If the bias is zero at some time \( t_0 \), it is then significantly more likely to be zero again at some later time than if the bias had been large at \( t_0 \). So as \( \langle \langle \tau^z(t) \rangle \rangle_{\xi} \) can change via tunneling, \( \langle \langle \tau^z(s_1) \rangle \rangle_{\xi} \) is correlated with \( \cos \left( \int_{s_1}^t ds_2 \xi(s_1) \right) \) and that correlation grows as \( t \) increases, making the approximation (6.63) invalid over long times.

So far we have calculated features of the model with diffusing bias in the limit where the diffusion is fast compared to the tunneling time scale. We could obtain further results for other regimes in this model. Instead as we are mainly interested in the dynamics of entanglement of the system with a bath, which is not captured in this model, we note the salient features of this model in the regime we have discussed and move on. We see that in this model in the regime studied \( \langle \langle \tau^x \rangle \rangle_{\xi} \) decays rapidly at a time scale set by the \( \Lambda^{-1} \). \( \langle \langle \tau^z \rangle \rangle_{\xi} \) decays over a larger time scale that depends on both the tunneling amplitude \( \Delta_0 \) and \( \Lambda \). \( \langle \langle \tau^y \rangle \rangle_{\xi} \) is approximately the sum of two components, a component that decays rapidly on the fast time scale \( \Lambda^{-1} \) and a component that decays on the slower timescale which comes from coherent oscillations around the \( x \).

### 6.4 Conclusion

In this chapter we have explore some simple models of the interaction of a central qubit coupled to an environment.
We have derived new results for correlators between the central qubit and spin bath in the degeneracy blocking model in section 6.1 and we have seen that information lost by the central qubit is transferred to higher and higher order correlations with bath spins. In chapter 7 will provide evidence for a similar cascade in a model of precessional decoherence, where the bath spins are allowed to flip.

In section 6.2 we derived methods for dealing with qubits under the influence of a dynamic bias. Finally in section 6.3 we study the effect of time dependent random bias acting on a qubit and saw some of the subtiles involved in using the equations of motion, when different components evolve on different different timescales.
Chapter 7

The Spin Bath Influence Functional and Precessional Decoherence

We now derive an influence functional approach to the motion of a system of central qubits coupled to a bath, analogous to that discussed in section 1.7.1 for the oscillator bath. This is a complementary approach to the hierarchy of equations of motion. The form of the spin bath influence functional that we derive is well suited to studying systems with a well defined discreet classical Hamiltonian and few different possible transitions or “jumps” which can occur.

We then use the influence functional to re-derive and extend the results obtained by Prokof’ev and Stamp [86], for precessional decoherence. In order to understand the dynamics of decoherence we calculate evolution of correlations between the central qubit and the bath spins in this model.

7.1 The Influence Function for Qubit Systems Coupled to a Spin Bath

Consider the case in section 1.7.2 were we have a set of system spins and bath spins governed by the Hamiltonian,

\[ H = \frac{1}{2} \sum_{a=1}^{N_S} h_a \cdot \tau_a + \frac{1}{2} \sum_{a \neq b}^{N_B} u_{\mu \nu}^{ab} \tau_a^{\mu} \tau_b^{\nu} + \frac{1}{2} \sum_{j=1}^{N_B} b_j \cdot \sigma_j + \frac{1}{2} \sum_{a} \sum_{j} V_{\mu \alpha}^{aj} \tau_a^{\mu} \sigma_j^{\alpha}. \]  

(7.1)

Now we chose the “classical” basis of the total Hilbert space in terms of a list of the classical values of the qubits \( s = (s_1, s_2, \ldots, s_{N_S}), \eta = (\eta_1, \eta_2, \ldots, \eta_{N_B}) \) are binary values \( s_a, \eta_i = \pm 1 \) so that our kets are

\[ |s \eta\rangle \equiv \prod_{a \in S} |s_a\rangle \prod_{i \in B} |\eta_i\rangle. \]  

(7.2)

It is then natural to split the Hamiltonian into parts \( H = H_\parallel + H_\perp \) which are diagonal \( H_\parallel \) in and completely off diagonal \( H_\perp \) in this basis. For the Hamiltonian
(7.1) we have

\[ H_\parallel = \frac{1}{2} \sum_{a=1}^{N_S} h^z_a \tau^z_a + \frac{1}{2} \sum_{a} \sum_{b \neq a} u_{ab}^{\tau^z_a \tau^z_b} + \frac{1}{2} \sum_{j=1}^{N_S} b^z_j \sigma^z_j + \frac{1}{2} \sum_{a} \sum_{j} V^{\tau^z_a \sigma^z_j} \]

(7.3)

\[ H_\perp = H - H_\parallel. \]

(7.4)

\[ |s\eta\rangle \text{ is by construction an eigenstate of } H_\parallel \text{ with an eigenvalue } h^0_s \text{ which is a classical energy associated with the classical bit configuration,} \]

\[ h^0_s \equiv \frac{1}{2} \sum_{a=1}^{N_S} h^z_a s^a \]

(7.5)

\[ h^{SB}_s \equiv \frac{1}{2} \sum_{j=1}^{N_B} b^z_j \eta^j + \frac{1}{2} \sum_{a} \sum_{j} V^{\tau^z_a \sigma^z_j} \]

(7.6)

Where as \( H_\perp \) defines a set of possible “jumps” or more precisely transition amplitudes between different states in the \( \{|s\eta\rangle\} \) basis. We now proceed to derive the influence functional. Start by defining the complete set of projectors \( p_{s\eta} \),

\[ p_{s\eta} = |s\eta\rangle \langle s\eta| \]

(7.7)

For each configuration of \( s\eta \) the projection operator \( p_{s\eta} \) projects onto a distinct orthogonal direction in Hilbert space, so we have the following completeness and orthogonality conditions

\[ p_{s\eta} p_{s'\eta'} = \delta_{ss'} \delta_{\eta\eta'} \]

(7.9)

\[ \sum_{s} \sum_{\eta} p_{s\eta} = 1 \]

(7.10)

and we can write the diagonal Hamiltonian and the associated evolution operator \( U_0(t, t') = e^{-iH_\parallel(t-t')} \) as

\[ H_\parallel = \sum_{s} \sum_{\eta} h^0_s p_{s\eta} \]

(7.11)

\[ H_\perp = \sum_{s} \sum_{\eta} \sum_{\eta'} \sum_{\eta''} p_{s\eta'} H_\perp p_{s\eta''} \]

(7.12)

\[ U_0(t, t') = \sum_{s} \sum_{\eta} e^{-i h^0_s (t-t')} p_{s\eta}. \]

(7.13)
Then expanding in the usual way the Dyson series [91] for the evolution operator in powers off diagonal Hamiltonian

\[
U(t) = \sum_{n=0}^{\infty} \sum_{\{\eta, \bar{\eta}\}} \left( \int_{0}^{t} dt_{n} \cdots \int_{0}^{t_{2}} dt_{1} \right) \exp \left\{ -i \sum_{\ell=0}^{n} (t_{\ell+1} - t_{\ell}) h_{\eta, \bar{\eta}} \right\} \tag{7.14}
\]

where \( t_{n+1} = t \) in each term in the sum \((7.14)\). We can interpret the expression for the evolution operator \((7.14)\) as a “sum over all paths” expression, here the paths consists of transitions contained in \(H_{\perp}\) between different states of the form \(|s\eta\rangle\), at times \(\{t_{\ell}\}\), with accumulation of phase according to \(H_{\parallel}\) in the time between the transitions events. Now one can use the expression \((7.14)\) to derive an expression for the elements of the system reduced density matrix \(\hat{\rho}_{S}^{\perp}(t) = \langle \bar{s}|\rho_{S}|s\rangle\) in terms of the initial full density matrix \(\rho(0)\)

\[
\hat{\rho}_{S}^{\perp}(t) = \sum_{n=0}^{\infty} \sum_{\{\eta, \bar{\eta}\}} \sum_{\{\tilde{\eta}, \bar{\tilde{\eta}}\}} \left( \int_{0}^{t} dt_{n} \cdots \int_{0}^{t_{2}} dt_{1} \int_{0}^{t} d\tilde{t}_{n} \cdots \int_{0}^{t_{2}} d\tilde{t}_{1} \right) \exp \left\{ -i \sum_{\ell=0}^{n} (t_{\ell+1} - t_{\ell}) h_{\eta, \bar{\eta}} + i \sum_{\ell=0}^{\tilde{n}} (\tilde{t}_{\ell+1} - \tilde{t}_{\ell}) h_{\tilde{\eta}, \bar{\tilde{\eta}}} \right\} \langle s|\rho_{S}\rangle \langle \bar{s}|p_{\eta, \bar{\eta}} H_{\perp} p_{\eta, \bar{\eta}} H_{\perp} \cdots p_{\eta, \bar{\eta}} H_{\perp} p_{\eta, \bar{\eta}} \rangle \tag{7.15}
\]

We will refer to \((7.15)\) as the transition expansion for the system reduced density matrix, it involves the sum of two sets of possible paths one with the system evolving forward in time with transitions occurring at the times \(\{t_{\ell}\}\) and the other evolving backwards in time with transitions occurring at the times \(\{\tilde{t}_{\ell}\}\).

The transition expansion expression for \(\hat{\rho}_{S}\) can be made to look a bit more like the influence functional expressions obtained when there is an oscillator bath. We split the projection operators \(p_{\eta, \bar{\eta}} = p_{S}^{B} p_{\eta, \bar{\eta}} \) into parts acting on the bath \(p_{\eta, \bar{\eta}}^{B} = |\eta\rangle\langle \eta|\) and central system \(p_{S}^{B} = |s\rangle\langle s|\). Then we assume that the off diagonal Hamiltonian can be written as a sum of products between system “transition” operators \(\{\tilde{t}_{a}\}\) and bath “transition” operators \(\{\tilde{T}_{a}\}\)

\[
H_{\perp} = \sum_{a} \tilde{t}_{a} \tilde{T}_{a} \tag{7.16}
\]

Note “transition” appeared in quotation marks in that last sentence because the way we have defined it \(H_{\perp}\) may have terms that only cause transitions either the
system or bath. Then if we assume that the initial density matrix is separable, \( \rho(0) = \hat{\rho}_S(0) \hat{\rho}_B(0) \), we can write the transition expansion (7.15),

\[
\rho_{SB}(t) = \sum_{n=0}^{\infty} \sum_{\tilde{n}=0}^{\infty} \sum_{\{a_\ell\}} \sum_{\{\tilde{a}_\ell\}} \left( \int_0^t dt_n \cdots \int_0^t dt_1 \int_0^t d\tilde{t}_n \cdots \int_0^t d\tilde{t}_1 \right) \exp \left\{ -i \sum_{\ell=0}^n (t_{\ell+1} - t_\ell) \hat{h}_{2\ell}^0 + i \sum_{\tilde{\ell}=0}^{\tilde{n}} (\tilde{t}_{\tilde{\ell}+1} - \tilde{t}_{\tilde{\ell}}) \hat{h}_{2\tilde{\ell}}^0 \right\} F \left[ s(t), \tilde{s}(\tilde{t}) ; \{a_\ell\}, \{\tilde{a}_\ell\} \right]
\]

(7.17)

where \( F \left[ s(t), \tilde{s}(\tilde{t}) ; \{a_\ell\}, \{\tilde{a}_\ell\} \right] \) is a functional of the two paths for the spin variables \( s(t) \), \( \tilde{s}(\tilde{t}) \) by the transition times \( \{t_\ell\} \), \( \{\tilde{t}_{\tilde{\ell}}\} \) and the values \( \{s_\ell\}, \{\tilde{s}_{\tilde{\ell}}\} \) in between the transitions, so

\[
\begin{align*}
    s(t) & = \{s_\ell\} \quad \text{for } t_{\ell-1} < t < t_\ell \quad (\forall \ell = 1, \ldots, n) \\
    \tilde{s}(\tilde{t}) & = \{\tilde{s}_{\tilde{\ell}}\} \quad \text{for } \tilde{t}_{\tilde{\ell}-1} < \tilde{t} < \tilde{t}_{\tilde{\ell}} \quad (\forall \tilde{\ell} = 1, \ldots, \tilde{n}).
\end{align*}
\]

(7.18)

The influence functional also depends on the sequences of different parts of the off diagonal Hamiltonian that result in these paths, specified by \( \{a_\ell\} \), \( \{\tilde{a}_\ell\} \). The influence functional is,

\[
F \left[ s(t), \tilde{s}(\tilde{t}) ; \{a_\ell\}, \{\tilde{a}_\ell\} \right] = \sum_{\{y_\ell\}} \sum_{\{\tilde{y}_{\tilde{\ell}}\}} \exp \left\{ -i \sum_{\ell=0}^n (t_{\ell+1} - t_\ell) \hat{h}_{2\ell}^{SB} + i \sum_{\tilde{\ell}=0}^{\tilde{n}} (\tilde{t}_{\tilde{\ell}+1} - \tilde{t}_{\tilde{\ell}}) \hat{h}_{2\tilde{\ell}}^{SB} \right\}
\]

(7.20)

\[
\left\langle \eta_n | \hat{T}_{a_n} \hat{p}^B_{\tilde{a}_{n-1}} \cdots \hat{T}_{a_1} \hat{p}^B_{\tilde{a}_1} \hat{T}_{a_0} \hat{p}^B_{\tilde{a}_0} \hat{\rho}_B(0) - \hat{p}^B_{\tilde{a}_0} \hat{T}_{a_0} \cdots \hat{p}^B_{\tilde{a}_1} \hat{T}_{a_1} \hat{p}^B_{\tilde{a}_{n-1}} | \eta_n \right\rangle.
\]

In general transition expansion is a complicated expression for the time evolution of the reduced density matrix or influence functional. The complexity of the different sums depend on the off diagonal part of the Hamiltonian (indeed when \( H_\perp = 0 \) the expression is trivial) which specifies all possible transitions. A strategy that can make the transition expansion manageable is to identify which sets of transitions are most important to the coherent evolution of the density matrix and then work with this reduced set of possible transitions, while either ignoring those that are less important or including them perturbatively. We will take this approach in the next section using the specific example of the precessional decoherence problem introduced in section 1.7.2.
7.2 Evaluating the Influence Functional for Precessional Decoherence

Consider the precessional decoherence model discussed in section 1.7.2 with a single central spin. The central spin has a purely longitudinal $\omega_i^\parallel$ coupling to bath spins $\{\sigma_i\}$, the bath spins and the central spins both have transition amplitudes $\Delta_0$ and $-i\omega_i^\perp$ (we have rotated our frame, from that in section 1.7.2). We assume that the transition amplitudes for the bath spins are small.

$$H = \frac{1}{2} \Delta_0 \tau^x + \frac{1}{2} \xi_0 \tau^z - \frac{1}{2} \sum_{i \in B} \omega_i^\parallel \sigma_i^z + \frac{1}{2} \sum_{i \in B} \omega_i^\perp \sigma_i^x \tau^z$$

(7.21)

$$\equiv \frac{1}{2} \Delta_0 \tau^x + \frac{1}{2} \xi_0 \tau^z + \sum_{i \in B} \tilde{B}_i$$

(7.22)

The precessional decoherence Hamiltonian is more complicated than the simple degeneracy blocking Hamiltonian discussed in the chapter 6, in the processional case the energy splitting of the central spin is no longer static as the bath spins can flip. So each transition in the transition expansion the central spin or any of the bath spins may flip making the expansion in its most straightforward form unwieldy. However there is a transformation which simplifies things considerably for this case.

7.2.1 Canonical Transformation of the Bath Spin Variables

The part of the Hamiltonian $\tilde{B}_i$ which acts on a single bath spin $i$ may be written

$$\tilde{B}_i = \frac{1}{2} \tau^z \left( \omega_i^\parallel \sigma_i^z - \omega_i^\perp \tau^z \sigma_i^y \right) = \frac{1}{2} \omega_i e^{-\frac{i}{2} \beta_i \tau^x \sigma_i^x} e^{\frac{i}{2} \beta_i \tau^x \sigma_i^x}$$

(7.23)

with $\{\beta_i\}$ are simply the angles defined in section 1.7.2

$$\omega_i \cos \beta_i = \omega_i^\parallel$$

(7.24)

$$\omega_i \sin \beta_i = \omega_i^\perp.$$  

(7.25)

Thus $\tilde{B}_i$ may be viewed as a longitudinal coupling in a frame where the bath spins are rotated by an angle depending on the central spins state. Hamiltonian can then be written

$$H = \frac{1}{2} \Delta_0 \tau^x + \frac{1}{2} \tilde{U}^\dagger \left( \xi_0 \tau^z + \sum_i \omega_i \tau^z \sigma_i^z \right) \tilde{U}$$

(7.26)

where

$$\tilde{U} \equiv \prod_{i \in B} e^{\frac{i}{2} \beta_i \sigma_i^x \tau^z}$$

(7.27)

(not be confused with $U(t)$ the evolution operator). Now perform a canonical transformation on Hilbert space $|\psi\rangle_{(\text{old})} \rightarrow \tilde{U} |\psi\rangle_{(\text{new})}$ then the Hamiltonian in this new
basis is
\[ H = \frac{1}{2} \Delta_0 \tilde{U} \tau^z \tilde{U}^\dagger + \frac{1}{2} \xi_0 \tau^z + \frac{1}{2} \sum_i \omega_i \tau^z \sigma_i^z. \] (7.28)

In this new basis the transformed Hamiltonian \((7.28)\) action of the off diagonal part of the Hamiltonian \(H_\perp = \frac{1}{2} \Delta_0 \tilde{U} \tau^z \tilde{U}^\dagger\) *always* flips the central spin. So that the new bath spins variables only flip when the central spin also flips. This will help when using the transition expansion for the reduced density matrix of the central spin.

The off diagonal part of the Hamiltonian can be written in a more intuitive form using the “ladder” operators \(\tau^\pm = |\pm 1\rangle \langle \mp 1|\):
\[ H_\perp = \frac{1}{2} \Delta_0 \tau^+ e^{i \sum_{i \in B} \beta_i \sigma_i^x} + \frac{1}{2} \Delta_0 \tau^- e^{-i \sum_{i \in B} \beta_i \sigma_i^x} \] (7.29)
\[ = \frac{1}{2} \Delta_0 \tau^+ \sum_{C \subseteq B} i^{|C|} \prod_{j \notin C} \cos \beta_j \prod_{i \in C} \sin \beta_i \sigma_i^x + \text{h.c.} \] (7.30)

Equations \((7.29)\) and \((7.30)\) can be interpreted as follows, the terms that flip of the central spin rotate the bath spins around their \(x\) axis in either the positive or negative orientation depending on the initial state of the central spin. As such the transition Hamiltonian contains terms that co-flip any number of bath spins with a central spin with amplitudes depending on the angles \(\{\beta_i\}\). Also, as there are off diagonal interaction terms in \((7.30)\) containing products of Pauli operators belonging to all subsets of the spin bath, the hierarchy of equations of motion for the qubits in this basis will link all orders of correlators, making the hierarchy less useful in this transformed basis.

### 7.2.2 The Orthogonality Blocking Approximation.

Now we describe an approximation first presented by Prokof’ev and Stamp \[86, 88\], which will reduce the number of components of \(H_\perp\) that we need to consider. We start with a mathematical explanation of this approximation before returning to a physical motivation. Begin by writing the transition expansion for the evolution operator \((7.14)\) for this case in the slightly different form
\[ U(t) = \sum_{n=0}^{\infty} \sum_{\{\eta_\ell\}} \left( \int_0^t dt_n \cdots \int_0^{t_2} dt_1 \right) \exp \left\{ -i \frac{h}{2} \sum_{\ell=1}^{n} t_\ell (\xi_\eta_{\ell-1} s_{\ell-1} - \xi_{\eta,\ell} s_\ell) \right\} \] (7.31)

where
\[ p_{z_n, y_n} H_\perp p_{z_{n-1}, y_{n-1}} H_\perp \cdots p_{z_1, y_1} H_\perp p_{z_0, y_0}, \]
\[ \xi_{\eta,\ell} \equiv \xi_0 + \sum_i \omega_i \eta_i, \] (7.32)

is the bath spin dependent bias on the central spins. Equation \((7.31)\) can be viewed as a perturbation expansion in \(H_\perp\) or equivalently in \(\Delta_0\). In such an expansion the terms can be classed as either secular or non-secular \[7\]. The secular terms diverge.
as some power of $t$ as $t \to \infty$, while the non-secular terms remain bounded for all $t$. The secular terms occur when one of the $dt_\ell$ integrals has an integrand with a zero frequency component. One can obtain an approximation which is valid for long times by summing all the most secular terms for every order of $\Delta_0$. That is keeping the terms in the series (7.31) in which the frequency is zero in every integrand, viz,

$$
\xi_{\ell-1} s_{\ell-1} = \xi_\ell s_{\ell},
$$

(7.33)

for all $\ell$, this is the orthogonality blocking approximation. Physically this amounts to keeping only transitions between resonant levels of $H_\|$, as these are the dominant transitions. Before we explore fully the validity of this approximation and use it to calculate the systems reduced density matrix we will specify some details involved in problem.

### 7.2.3 Calculation of the Reduced Density Matrix

Before completing the calculation we need to specify the initial density matrix and parameters.

For simplicity we will assume that the bias field $\xi_0 = 0$, so that all the bias comes from the bath spins. We will also assume the couplings can be written as,

$$
\omega_j = \omega_0 + \delta \omega_j,
$$

(7.34)

and are some small deviation $\delta \omega_j$ from a mean value of $\omega_0$. We begin by assuming $\delta \omega_j = 0$ for simplicity.

We assume the system and the bath are in a product state to begin with so that $\rho(0) = \rho_S(0)\rho_B(0)$, where the initial state for the central system is some arbitrary pure state $\rho_S(0)$ which has been prepared by some process. Furthermore assume that as the bath spins do not interact directly, the bath initial state is a product state $\rho_B(0) = \prod_{i \in B} \tilde{\rho}_i(0)$ where $\tilde{\rho}_i(0) = |\pm_1\rangle \langle \pm_1|$. We will make the further assumption that the number of bath spins which are initially up and the number which are initially down are equal. This along with the $\xi_0$ assumption corresponds to operating the qubit at its so called “sweet spot”, where the rate of change of the central qubit energy with $\xi$ is zero. Operating qubits at such a point is a commonly used method to prevent decoherence, see for example [55, 97, 106, 112].

The fact that we are working in a basis which is transformed from the physical bath states complicates things a little here but we assume that the central spin state is prepared in such a way that the separation in the transformed basis is nearly exact. We will consider the effect of relaxing this approximation later.
As discussed earlier the amplitude for flipping the bath spins is much less than the coupling to the central spin \( b_i^\perp \ll \omega_i^\parallel \) so that \( \beta_i \ll 1 \). This allows for a large variety of transitions which still satisfy the orthogonality blocking condition \( \xi_{j_{\perp} i} s_{\ell - 1} = \xi_{j_{\perp} i} s_{\ell} \). In this case we will see the orthogonality blocking approximation will give us the leading term in an expansion for the dynamics in the small parameter \( \beta_i \).

With the above assumptions and initial conditions in mind we find that the orthogonality blocking approximation just means that between each central spin flip the bath is in the zero polarisation group. So that the only relevant part of the off diagonal Hamiltonian is

\[
H_\perp \rightarrow \frac{1}{2} \Delta_0 \tau^+ \mathcal{P}_0 e^{i \sum_{i \in B} \beta_i \sigma^i} \mathcal{P}_0 + \frac{1}{2} \Delta_0 \tau^- \mathcal{P}_0 e^{i \sum_{i \in B} \beta_i \sigma^i} \mathcal{P}_0 \tag{7.35}
\]

where \( \mathcal{P}_0 \) is the projection operator that projects the bath onto the zero magnetisation polarisation group. \( \mathcal{P}_0 \) can be written

\[
\mathcal{P}_0 = \int_0^{2\pi} \frac{d\xi}{2\pi} \exp \left( i \sum_{i \in B} \xi \sigma^i \right). \tag{7.36}
\]

Now one can employ the transition expansion (7) to obtain an expression for the reduced density matrix of the central system, which can be specified with the correlators

\[
\langle \tau^+ (t) \rangle = \sum_{n=0}^{\infty} \left\{ \frac{(-i \Delta_0 t)^{2n}}{(2n)!} \left[ \langle \tau^- \rangle A_{\perp \perp}^{(n)} + \langle \tau^+ \rangle A_{\perp \perp}^{(n)} \right] \right. \\
+ \left. \frac{(-i \Delta_0 t)^{2n+1}}{(2n+1)!} \left[ \frac{1}{2} (1 + \langle \tau^z \rangle) A_{\perp \perp}^{(n)} + \frac{1}{2} (1 - \langle \tau^z \rangle) A_{\perp \perp}^{(n)} \right] \right\} \tag{7.37}
\]

\[
\langle \tau^- (t) \rangle = \sum_{n=0}^{\infty} \left\{ \frac{(-i \Delta_0 t)^{2n}}{(2n)!} \left[ \langle \tau^- \rangle A_{\perp \perp}^{(n)} + \langle \tau^+ \rangle A_{\perp \perp}^{(n)} \right] \right. \\
+ \left. \frac{(-i \Delta_0 t)^{2n+1}}{(2n+1)!} \left[ \frac{1}{2} (1 + \langle \tau^z \rangle) A_{\perp \perp}^{(n)} + \frac{1}{2} (1 - \langle \tau^z \rangle) A_{\perp \perp}^{(n)} \right] \right\} \tag{7.38}
\]

\[
\langle \tau^z (t) \rangle = \sum_{n=0}^{\infty} \left\{ \frac{(-i \Delta_0 t)^{2n}}{(2n)!} \left[ \frac{1}{2} (1 + \langle \tau^z (0) \rangle) A_{\perp \perp}^{(n)} + (1 - \langle \tau^z (0) \rangle) A_{\perp \perp}^{(n)} \right] \right. \\
+ \left. \frac{(-i \Delta_0 t)^{2n+1}}{(2n+1)!} \left[ \langle \tau^+ (0) \rangle A_{\perp \perp}^{(n)} + \langle \tau^- (0) \rangle A_{\perp \perp}^{(n)} \right] \right\} - \frac{1}{2}. \tag{7.39}
\]

Here the quantities \( A_{\mu \nu}^{(n)} \) are sums of influence functionals for the spin bath with the same numbers of flips of the central spin where the central spins path has the same
end points, mathematically

\[
A_{-+}^{(n)} = \frac{1}{2^{2n}} \sum_{\ell=0}^{n} \binom{2n}{2\ell} \left\langle \left( \mathcal{P}_0 U^\dagger \mathcal{P}_0 \right)^\ell \left( \mathcal{P}_0 U \mathcal{P}_0 U^\dagger \right)^{n-\ell} \right\rangle 
\]

\[
A_{++}^{(n)} = -\frac{1}{2^{2n}} \sum_{\ell=0}^{n-1} \binom{2n}{2\ell+1} \left\langle \left( \mathcal{P}_0 U \mathcal{P}_0 U^\dagger \right)^\ell \left( \mathcal{P}_0 U \mathcal{P}_0 U^\dagger \right)^{n-\ell} \mathcal{P}_0 U \right\rangle 
\]

\[
A_{+\uparrow}^{(n)} = -\frac{1}{2^{2n+1}} \sum_{\ell=0}^{n} \binom{2n+1}{2\ell+1} \left\langle \left( \mathcal{P}_0 U^\dagger \mathcal{P}_0 \right)^\ell \left( \mathcal{P}_0 U^\dagger \mathcal{P}_0 \right)^{n-\ell} \mathcal{P}_0 \right\rangle 
\]

\[
A_{-\downarrow}^{(n)} = -\frac{1}{2^{2n+1}} \sum_{\ell=0}^{n} \binom{2n+1}{2\ell+1} \left\langle \left( \mathcal{P}_0 U \mathcal{P}_0 U^\dagger \right)^\ell \left( \mathcal{P}_0 U \mathcal{P}_0 U^\dagger \right)^{n-\ell} \mathcal{P}_0 \right\rangle 
\]

\[
A_{-\uparrow}^{(n)} = -\frac{1}{2^{2n+1}} \sum_{\ell=0}^{n} \binom{2n+1}{2\ell+1} \left\langle \left( \mathcal{P}_0 U \mathcal{P}_0 U^\dagger \right)^\ell \left( \mathcal{P}_0 U^\dagger \mathcal{P}_0 \right)^{n-\ell} \mathcal{P}_0 \right\rangle 
\]

\[
A_{+\downarrow}^{(n)} = \frac{1}{2} \left\langle \left( \mathcal{P}_0 U^\dagger \mathcal{P}_0 \right)^n \right\rangle 
\]

\[
A_{+\uparrow}^{(n)} = -\frac{1}{2} \left\langle \left( \mathcal{P}_0 U \mathcal{P}_0 U^\dagger \right)^n \right\rangle 
\]

\[
A_{-\uparrow}^{(n)} = \frac{1}{2} \left\langle \left( \mathcal{P}_0 U^\dagger \mathcal{P}_0 \right)^n \mathcal{P}_0 \right\rangle 
\]

\[
A_{-\downarrow}^{(n)} = -\frac{1}{2} \left\langle \mathcal{P}_0 U \left( \mathcal{P}_0 U \mathcal{P}_0 U^\dagger \right)^n \right\rangle 
\]

Here \( \binom{n}{\ell} = \frac{n!}{\ell!(n-\ell)!} \) is the binomial coefficient, \( U = U(\{\beta_i\}) \) is the unitary rotation

\[
U(\{\beta_i\}) \equiv e^{i \sum_j \beta_j \sigma^j}, \quad (7.52)
\]

and all the averages are traces over the bath, \( \langle \ldots \rangle = \text{tr}_B(\ldots \hat{\rho}_B(0)) \). Now the problem of the calculation of the reduced density matrix is reduced to averaging factors that depend on expectations of strings of operators acting on the bath space. Prokef'ev and Stamp \cite{86} used this approximation to compute the return probability \( p_{r0}(t) \) for the central spin when it is initially polarised in the up direction. We will present this calculation here and then show that the results obtained by Prokef'ev and Stamp
can be generalised to arbitrary initial conditions.
From equation (7.39) we have
\[ p_{\tau_0}(t) = \frac{1}{2} (1 + \langle \tau_z(t) \rangle) = \sum_{n=0}^{\infty} \frac{(-i\Delta_0 t)^{2n}}{(2n)!} \frac{1}{2} \left\langle \left( \Psi_0 U^\dagger \Psi_0 U \right)^n \right\rangle. \] (7.53)

The expectation appearing in this expression can be factorised using the representation (7.36) for the projection operators,
\[
\left\langle \left( \Psi_0 U^\dagger \Psi_0 U \right)^n \right\rangle = \int_0^{2\pi} \frac{d^{2n} \xi}{(2\pi)^{2n}} \prod_{i \in B} \left( e^{i\xi_1 \sigma_i^r} e^{-i\beta_i \sigma_i^z} e^{i\xi_2 \sigma_i^r} e^{i\beta_i \sigma_i^z} \right) e^{i\xi_3 \sigma_i^r} e^{-i\beta_i \sigma_i^z} e^{i\xi_4 \sigma_i^r} e^{i\beta_i \sigma_i^z} \ldots \left( e^{i\xi_{2n-1} \sigma_i^r} e^{-i\beta_i \sigma_i^z} e^{i\xi_{2n} \sigma_i^r} e^{i\beta_i \sigma_i^z} \right). \] (7.54)

So we need to approximate each of these factors. If \( i \) is a bath spin which is initially up, then one has
\[
\left\langle e^{i\xi_1 \sigma_i^r} e^{-i\beta_i \sigma_i^z} e^{i\xi_2 \sigma_i^r} e^{i\beta_i \sigma_i^z} \right\rangle \left( e^{i\xi_3 \sigma_i^r} e^{-i\beta_i \sigma_i^z} e^{i\xi_4 \sigma_i^r} e^{i\beta_i \sigma_i^z} \right) \ldots \left( e^{i\xi_{2n-1} \sigma_i^r} e^{-i\beta_i \sigma_i^z} e^{i\xi_{2n} \sigma_i^r} e^{i\beta_i \sigma_i^z} \right) = e^{i \sum_{\ell} \xi_{\ell}} \left( 1 - n_\beta_i \beta_i^2 + \sum_{\ell=1}^{2n-1} \sum_{\ell' = \ell+1}^{2n} (-1)^{\ell + \ell'} e^{-2i \sum_{\ell = \ell+1}^{\ell'} \xi_i} + O(\beta_i^3) \right) = \exp \left\{ i \sum_{\ell} \xi_{\ell} - n_\beta_i \beta_i^2 + \sum_{\ell=1}^{2n-1} \sum_{\ell' = \ell+1}^{2n} (-1)^{\ell + \ell'} e^{-2i \sum_{\ell = \ell+1}^{\ell'} \xi_i} \right\} + O(\beta_i^3). \] (7.55)

Similarly if \( j \) is a bath spin which is initially down, then one has
\[
\left\langle e^{i\xi_1 \sigma_j^r} e^{-i\beta_j \sigma_j^z} e^{i\xi_2 \sigma_j^r} e^{i\beta_j \sigma_j^z} \right\rangle \left( e^{i\xi_3 \sigma_j^r} e^{-i\beta_j \sigma_j^z} e^{i\xi_4 \sigma_j^r} e^{i\beta_j \sigma_j^z} \right) \ldots \left( e^{i\xi_{2n-1} \sigma_j^r} e^{-i\beta_j \sigma_j^z} e^{i\xi_{2n} \sigma_j^r} e^{i\beta_j \sigma_j^z} \right) = \exp \left\{ -i \sum_{\ell} \xi_{\ell} - n_\beta_j \beta_j^2 + \sum_{\ell=1}^{2n-1} \sum_{\ell' = \ell+1}^{2n} (-1)^{\ell + \ell'} e^{2i \sum_{\ell = \ell+1}^{\ell'} \xi_i} \right\} + O(\beta_j^3). \] (7.56)
Therefore
\[
\left\langle \left( \mathcal{P}_0 U \mathcal{P}_0 U^\dagger \right)^n \right\rangle \approx \int_{0}^{2\pi} \frac{d^{2n} \xi}{(2\pi)^{2n}} \exp \left\{ -n \sum_{i \in \mathcal{B}} \beta^2_i - \sum_{i \in \mathcal{B}} \beta^2_i \sum_{\ell = 1}^{2n-1} \sum_{\ell' = \ell}^{2n} (-1)^{\ell + \ell'} e^{2\pi i \sum_{\ell = \ell+1}^\ell \xi_i} \right\}
\]
\[
= \int_{0}^{2\pi} \frac{d^{2n} \xi}{(2\pi)^{2n}} \exp \left\{ -n N \beta^2 - N \beta^2 \sum_{\ell = 1}^{2n-1} \sum_{\ell' = \ell+1}^{2n} (-1)^{\ell + \ell'} \cos \left( 2 \sum_{\ell = \ell+1}^\ell \xi_i \right) \right\}.
\] (7.58)

Where we have assumed that the $\beta_i$ variables are sharply peaked around their mean $\beta_i \approx \beta \equiv \sum_i \beta_i/N$. Now with the substitution,
\[
\chi_\ell = 2 \sum_{\ell' = 1}^\ell \xi_{\ell'} + \ell \pi
\] (7.59)
we get
\[
\left\langle \left( \mathcal{P}_0 U \mathcal{P}_0 U^\dagger \right)^n \right\rangle = \int_{0}^{2\pi} \frac{d^{2n} \chi}{(2\pi)^{2n}} \exp \left\{ -n N \beta^2 - N \beta^2 \sum_{\ell = 1}^{2n-1} \sum_{\ell' = \ell+1}^{2n} \cos (\chi_\ell - \chi_{\ell'}) \right\}.
\] (7.60)

Which can be thought of as a partition function of $2n$ “classical pseudo-spins”, $\vec{s}_\ell = (\cos \chi_\ell, \sin \chi_\ell)$, defining $\vec{S} = \sum_\ell \vec{s}_\ell$, we have $\sum_{\ell = 1}^{2n-1} \sum_{\ell' = \ell+1}^{2n} 2 \cos (\chi_\ell - \chi_{\ell'}) + 2n = ||\vec{S}||^2 = S^2(\chi)$, so,
\[
\left\langle \left( \mathcal{P}_0 U \mathcal{P}_0 U^\dagger \right)^n \right\rangle = \int_{0}^{2\pi} \frac{d^{2n} \chi}{(2\pi)^{2n}} \exp \left\{ -N \beta^2 S^2(\chi) \right\}
\] (7.61)
\[
= \int d\vec{S} e^{-N \beta^2 S^2} \int_{0}^{2\pi} \frac{d^{2n} \chi}{(2\pi)^{2n}} \delta \left( \vec{S} - \sum_\ell \vec{s}_\ell \right)
\] (7.62)
\[
= \int \frac{dX}{2\pi} \int d\vec{S} e^{-N \beta^2 S^2 + iX \cdot \vec{S}} \left[ \int \frac{d\chi}{2\pi} e^{-iX \cdot \vec{s}_\ell} \right]^{2n}
\] (7.63)
\[
= \int_{0}^{\infty} dX \frac{X}{2\kappa} e^{-\frac{X^2}{4\pi \kappa}} J_0(X)^{2n}.
\] (7.64)

We denote an $n$’th order Bessel function of the first kind \cite{26} by $J_n(X)$. Inserting (7.64) into (7.53) we have
\[
\rho_{\text{r}}(t) = \int_{0}^{\infty} dX \frac{X}{2\kappa} e^{-\frac{X^2}{4\pi \kappa}} \frac{1}{2} \sum_{n=0}^{\infty} \frac{(-i \Delta_0 J_0(X) t)^{2n}}{(2n)!}.
\] (7.65)
The expression (7.65) is of the form of an average over the variable $X$, which enters into the motion through a renormalised transition element $\Delta(X) = \Delta_0 J_0(X)$. The averaged function (7.65) is exactly the value for the same probability $P_{\uparrow\uparrow}$, which we would calculate if the Hamiltonian was just $H_0(\Delta_0 J_0(X)) = \frac{1}{2} \Delta_0 J_0(X) \tau^x$. $X$ has a probability distribution function

$$P(X) = \frac{X}{2k} e^{-\frac{X^2}{4k^2}}, \quad (7.66)$$

the parameter $\kappa$ which controls the probability density of the average is

$$\kappa = \frac{1}{2} \sum_j \beta_j^2. \quad (7.67)$$

In order to generalise the calculation given above to the case where the central spin has arbitrary initial conditions and to calculate all the components of $\langle \tau(t) \rangle$ one needs to: (i) derive expressions analogous to (7.58) for all of the expectations appearing in equations (7.40-7.51). (ii) Transform the $\{\xi_q\}$ variables in the resulting expression to get an exponent which is manageable. This is done in appendix E.1.

The result in the lowest order orthogonality blocking approximation is that in order to calculate $\langle \tau(t) \rangle$ we need to perform the same averaging procedure, that is

$$\langle \tau(t) \rangle = \int_0^\infty dX X e^{-\frac{X^2}{2\kappa}} \langle \tau(t; \Delta_0 J_0(X)) \rangle_0, \quad (7.68)$$

where $\langle \tau(t; \Delta_0 J_0(X)) \rangle_0$ is the expectation of the central qubit polarisation calculated using the bare Hamiltonian $H_0(\Delta_0 J_0(X)) = \frac{1}{2} \Delta_0 J_0(X) \tau^x$.

The Decay of $\langle \tau^x(t) \rangle$

Now the equation (7.68) is unsatisfactory, as it it predicts that a central spin initialised in the state $\rho_S(0) = \frac{1}{2}(1 + \tau^x)$ should remain static. The reason for this can be understood physically. The most secular terms conserve the “longitudinal energy” $\sum_j \omega_j \tau^z \sigma^z_j$, which is initially zero. Thus the longitudinal energy term in the Hamiltonian, which changes the $x$ component of the central spin has no effect when only these terms are kept. Because of this we expect, something like we had in the example in section 6.3.2, one component of the central spin (in this case $\langle \tau^x \rangle$ and in the example, $\langle \langle \tau^z \rangle \rangle_{\xi}$) decays at a much slower rate that the other components and a higher order approximation is needed to calculate this decay.

In order to find any dynamics for $\langle \tau^x(t) \rangle$ for the Hamiltonian (7.26), one needs to go to a higher order in the orthogonality blocking approximation. The next lowest order approximation can be obtained by allowing two of the transitions which change the bath’s polarisation group, first jumping from its initial value and then on the second central spin flip, jumping back to its original value (transition sequences
with only one change in the polarisation group do not contribute to the dynamics of $\langle \tau \rangle$, as they give zero when we trace out the bath. We show in the appendix E.2 that this “next to leading order” orthogonality blocking approximation to $\langle \tau^x(t) \rangle$, gives zero (when we have the same parameters and initial conditions discussed in the previous section). This is because of a cancellation of the next to leading order terms, which relies on the initial state of the bath having zero $z$ magnetisation as well as zero external bias and so represents a somewhat special case. Rather than computing higher order terms in the transition expansion, we will briefly describe other effects which we have not included in the transition calculations so far, that can also cause $\langle \tau^x \rangle$ to evolve.

Small residual bias on the central qubit. Suppose the central qubit is imperfectly tuned to near its “sweet spot” and there is a small bias $\xi_0 \neq 0$ remaining on the central spin. Suppose that this is much less than the coupling between the bath and central spin ($\xi_0 \ll \omega_0$). In this case a single transition which flips the central spin, will not be able to satisfy the resonance condition \eqref{eq:resonance_condition} exactly, but we will still be able to obtain an approximation by satisfying these conditions approximately. In this approximation the mathematics used to evaluate the strings of operators appearing in equations \eqref{eq:bare_polarisation} to \eqref{eq:polarisation_time} is unaffected as an average, however between each central spin flip the density matrix is accumulating phase at a rate of $\pm \xi_0$ from the mismatched bias. Thus at time $t$ the central system polarisation will be

$$\langle \tau(t) \rangle = \int_0^\infty \mathrm{d}XXe^{-\frac{X^2}{4N\beta}} \langle \tau(t; J_0(X), \xi_0) \rangle_0,$$ \eqref{eq:polarisation_time}

where $\langle \tau(t; J_0, \xi_0) \rangle_0$ is the polarisation computed, from the “bare Hamiltonian” $H_0 \equiv \frac{1}{2}(\Delta_0 \tau^x + \xi_0 \tau^z)$. The averaging in equation \eqref{eq:polarisation_time} causes the decay of $\langle \tau^x \rangle$, because the small bias can rotate this component of the central polarisation into the $y-z$ plane, then the averaging over different transition amplitudes causes the decay.

Disorder in the coupling strengths, $\{\omega_j\}$. We relax the condition that all coupling strengths $\omega_j$ are the same by allowing them to each have a small deviation $\delta \omega_j$ from the mean (C.F. equation \eqref{eq:coupling_deviation}). In this case each polarisation group of the bath spins will have a range of energies. This will affect the dynamics in two ways, (i) there will be states with zero bath $z$ polarisation where the central spin still feels a non-zero bias, (ii) transitions which still approximately satisfy the resonance condition \eqref{eq:resonance_condition} can change the bias the central spin feels. If we assume for simplicity that the distribution of the couplings is approximately Gaussian with a small standard deviation $\delta \omega \ll |\omega_0|$, then distribution of possible biases felt by the central spin is as shown in figure 1.3 each polarisation group is spread out. In this case a typical bath state with zero polarisation has a bias on the central spin...
of order $\delta \omega / \sqrt{N}$ and an transition where this does not change is approximately on resonance. Thus when the variables $\beta_i$ are small the dominant transitions do not change the bias, so we expect the dynamics to be similar to those obtained with a small residual bias, described in the previous paragraph.

**Additional averaging over initial states.** One can expect the previous cases to cover a realistic experiment on a system described by the Hamiltonian (7.26). The bath starts in a definite pure state which only exerts a small bias on the central system. We will discuss in more detail the model with parameters suitable for realistic system of a single molecule magnet in chapter 8. However most experiments on such systems are performed on an ensemble of such systems. Even when studying a single system in order to reconstruct the full central system reduced density matrix, one needs to perform multiple experiments and in each of these experiments one does not have full control of the bath. In both of the cases the results of experiments will be an average over a set of initial bath configurations, much like in section 6.1. One can imagine a realistic case where the system is prepared with the bath in a zero polarisation group state for each run of the experiment, the central system polarisation vector recovered from such experiments will be an average of dynamics described in equation (7.69) over the probability distribution $P_0(\xi_0)$ for biases in this polarisation group,

$$
\langle \tau(t) \rangle = \int_{-\infty}^{\infty} d\xi_0 P_0(\xi_0) \int_{0}^{\infty} dX X e^{-\frac{X^2}{4N\beta}} \langle \tau(t; \Delta_0 J_0(X), \xi_0) \rangle_0,
$$

(7.70)

where $\langle \tau(t; \Delta_0, \xi_0) \rangle_0$ is the polarisation computed, from the “bare Hamiltonian” $H_0 \equiv \frac{1}{2}(\Delta_0 \tau^x + \xi_0 \tau^z)$.

### 7.2.4 Dynamics of Decoherence in the Canonical Variables

As in section 6.1.3 it is interesting to ask where the information lost by the central qubit goes. In particular we are interested whether the picture described in section 6.1.3 where information cascades from the central qubit to higher and higher order correlators with the bath, holds up when the bath spins can flip. In this section we explore this question.

When written in terms of the canonical variables the Hamiltonian (7.26) is no longer only contains local fields and pairwise interactions so the structure of the hierarchy of equations of motion will be much more complicated. In these canonical
variables the equation of motion for the central qubit polarization is

\[
\frac{d}{dt} \langle \tau \rangle = \frac{\Delta_0}{2} \left\{ i\langle (U - U^\dagger)\tau^z \rangle \dot{x} + \langle (U + U^\dagger)\tau^z \rangle \dot{y} \\
- \left[ i\langle (U - U^\dagger)\tau^x \rangle + \langle (U + U^\dagger)\tau^y \rangle \right] \dot{z} \right\} + \sum_j \omega_j \dot{z} \times \langle \tau \sigma^z_j \rangle. \tag{7.71}
\]

It follows from the orthogonality blocking approximation that the key terms in the decay of the central spin polarisation are those which involve correlations of \(U(\{\beta_i\})\) with the central spin. We have seen in equation (7.30) how terms involving \(U(\{\beta_i\})\) can be expressed as sums over clusters of bath spins of terms which depend on the \(x\) components of the bath spins in the cluster. So we expect the information lost by the central spin to be transferred into correlators between central spin components and operators like \(\prod_C \sigma^x_i\) for clusters \(C\) of bath spins. Now we move on to calculating some of these correlators.

We begin by considering all possible correlators between two or fewer bath spins and the central spin. We restrict ourselves to a central system intilised in the state \(\hat{\rho}_S(0) = |\uparrow\rangle \langle \uparrow|\). The details of all calculations in this section are contained in appendix E.3, here we describe how the calculations are done and the results. In the leading order orthogonality blocking approximation transition expansion the bath must end in the same polarisation group as it begins. This means that in this approximation any calculation of the expectation of an operator \(\hat{O}\), will result in an expression of the form

\[
\langle \hat{O}(t) \rangle = \text{tr} \left\{ \sum \ldots \hat{\rho}_0 \hat{O} \hat{\rho}_0 (\ldots) \rho(0) \right\}, \tag{7.72}
\]

where \((\ldots)\) represents terms omitted for clarity. Thus only operators whose action preserves the bath polarisation group contribute at the lowest order. Therefore the correlators \(\langle \tau^\mu \sigma^z_i \rangle = \langle \tau^\mu \sigma^y_i \rangle = 0\). In appendix E.3.2 we show that to leading order our expansion the correlators \(\langle \tau^\mu \sigma^z_i \rangle\) and \(\langle \tau^\mu \sigma^z_i \sigma^z_j \rangle\), which involve the \(z\) components of bath spins are,

\[
\langle \tau^\mu \sigma^z_i \rangle(t) = \eta_i \langle \tau^\mu \rangle(t) \tag{7.73}
\]

\[
\langle \tau^\mu \sigma^z_i \sigma^z_j \rangle(t) = \eta_i \eta_j \langle \tau^\mu \rangle(t). \tag{7.74}
\]

Therefore these correlators decay at the same rate as the associated central spin polarisation components. For the correlators of the form \(\langle \tau^\mu \sigma^x_i \sigma^x_j \rangle\), \(\langle \tau^\mu \sigma^y_i \sigma^y_j \rangle\), and \(\langle \tau^\mu \sigma^y_i \sigma^y_j \rangle\), which contain the transverse component of pairs of bath spins, however we get non-trivial results. This is important as these were precisely the correlators that we argued in the previous paragraph should contribute to the decay of the
central spin polarisation. The calculation of these correlators is in appendix \[E.3.1\], it is done as follows. Because $\sigma^x_j$ and $\sigma^y_j$ are off diagonal, bath spins $i$ and $j$ must flip along with one of the central spins flips to contribute to these correlators. The leading order calculation consists of summing a contribution from every central spin flip that these co-flips could coincide with. Naturally the result of this calculation depends on the initial state of the spins $i$ and $j$, as they can either be both initially up, down, or one may be up and the other down. In the case where both spins $i$ and $j$ are initially up (or down) we have the results,

\[
\langle \sigma^x_i \sigma^x_j \rangle = \langle \sigma^y_i \sigma^y_j \rangle = \beta_i \beta_j \left( \Delta_0 \right)^2 \int dXP(X) \left[ J_1(X) \right]^2 \tag{7.75}
\]

\[
\langle \sigma^z_i \sigma^x_j \rangle = \langle \sigma^x_i \sigma^y_j \rangle = \beta_i \beta_j \left( \Delta_0 \right)^2 \int dXP(X) \left[ J_1(X) \right]^2 \tag{7.76}
\]

\[
\langle \tau^x \sigma^x_i \sigma^y_j \rangle = \langle \tau^x \sigma^y_i \sigma^x_j \rangle = \langle \tau^x \sigma^y_i \sigma^y_j \rangle = \langle \tau^x \sigma^y_i \sigma^x_j \rangle = 0 \tag{7.77}
\]

\[
\langle \tau^y \sigma^x_i \sigma^x_j \rangle = \langle \tau^y \sigma^y_i \sigma^x_j \rangle = \langle \tau^y \sigma^y_i \sigma^y_j \rangle = \langle \tau^y \sigma^x_i \sigma^x_j \rangle \tag{7.78}
\]

\[
= \beta_i \beta_j \frac{\left( \Delta_0 \right)^2}{2} \int dXP(X) \left[ J_1(X) \right]^2 \sin[\Delta_0 J_0(X) t] \tag{7.79}
\]

\[
\langle \tau^y \sigma^x_i \sigma^y_j \rangle = \langle \tau^y \sigma^y_i \sigma^y_j \rangle = 0 \tag{7.80}
\]

\[
\langle \tau^z \sigma^x_i \sigma^x_j \rangle = \langle \tau^z \sigma^y_i \sigma^y_j \rangle \tag{7.81}
\]

\[
= - \beta_i \beta_j \frac{\left( \Delta_0 \right)^2}{4} \int dXP(X) \left[ J_1(X) \right]^2 \cos[\Delta_0 J_0(X) t] \tag{7.82}
\]

\[
\langle \tau^z \sigma^y_i \sigma^x_j \rangle = \langle \tau^z \sigma^x_i \sigma^y_j \rangle = 0. \tag{7.83}
\]
While if spin $i$ is initially up and spin $j$ is initially down we then have,

$$\langle \sigma^x_i \sigma^x_j \rangle = \langle \sigma^y_i \sigma^y_j \rangle = \frac{\Delta_0 t^2}{4} \int dXP(X) |J_1(X)|^2$$  \hspace{1cm} (7.82)

$$\langle \sigma^y_i \sigma^y_j \rangle = \langle \sigma^x_i \sigma^x_j \rangle = 0$$  \hspace{1cm} (7.83)

$$\langle \tau^z_i \sigma^x_i \sigma^x_j \rangle = \langle \tau^z_i \sigma^y_i \sigma^y_j \rangle = 0$$  \hspace{1cm} (7.84)

$$\langle \tau^z_i \sigma^x_i \sigma^y_j \rangle = - \langle \tau^z_i \sigma^y_i \sigma^x_j \rangle = \beta_i \beta_j \Delta_0 t \int dXP(X) J_0(X)$$  \hspace{1cm} (7.85)

$$\langle \tau^y_i \sigma^x_i \sigma^y_j \rangle = \langle \tau^y_i \sigma^y_i \sigma^y_j \rangle = 0$$  \hspace{1cm} (7.86)

$$\langle \tau^y_i \sigma^x_i \sigma^x_j \rangle = \langle \tau^y_i \sigma^y_i \sigma^y_j \rangle$$  \hspace{1cm} (7.87)

$$= - \beta_i \beta_j \int dXP(X) \left\{ \left[ \Delta_0 J_0(X) t \right] \cos[\Delta_0 J_0(X) t] \right\} \left\{ \left[ \Delta_0 J_0(X) t \right] \sin[\Delta_0 J_0(X) t] \right\}$$

$$\langle \tau^z_i \sigma^x_i \sigma^y_j \rangle = \langle \tau^z_i \sigma^y_i \sigma^x_j \rangle = 0$$\hspace{1cm} (7.88)

$$= \beta_i \beta_j \frac{1}{2} \int dXP(X) \left\{ \left[ \Delta_0 J_0(X) t \right] \sin[\Delta_0 J_0(X) t] \right\} \left\{ \left[ \Delta_0 J_0(X) t \right] \cos[\Delta_0 J_0(X) t] \right\}$$

$$\langle \tau^z_i \sigma^y_i \sigma^x_j \rangle = \langle \tau^z_i \sigma^x_i \sigma^y_j \rangle = 0.$$  \hspace{1cm} (7.89)

The first thing one should note about the results in equations (7.75-7.89), is that in both cases there are correlators which appear to diverge as $t \to \infty$. However this divergence is not a problem because our expansion is in small $(\beta_i \beta_j)$, is not valid for large $\beta_i \beta_j \Delta_0 t$ or large $\sqrt{\beta_i \beta_j \Delta_0 t}$.

The expressions for the non-zero correlators are all of the form, of an averaged expressions which grow over time a slow time scale depending on $\beta_i \beta_j$. In the case where both $i$ and $j$ are initially up (or down) the non-zero correlators (7.78) and (7.80), obtained when the two bath spins are aligned oscillate with amplitudes which grow quadratically with time. While in the case where the two bath spins are initially anti-aligned the correlators (7.86) and (7.88), have oscillating components that grow linearly with time as well as the quadratically growing components, while the correlators (7.85) grow linearly with time. This difference in scaling comes from the fact that, in the situation where the spins $i$ and $j$ are initially different, there is the possibility that both spins $i$ and $j$ may co-flip along with the same central spin flip. We also note that, as expected correlators of the form $\langle \tau^\mu \sigma^\nu_i \sigma^\rho_j \rangle$, which are important in the decay of the central spin, grow.

Interestingly equations (7.82) and (7.75) show, in both cases the two bath spins become correlated over time. This correlation increases quadratically and in the opposite sense in the two cases, initially aligned spins develop positive correlati-
ons between their $x$ components, while initially anti-aligned spins develop negative correlations between their $x$ components.

We have also calculated the correlators $\langle \tau^y \sigma_i^x \sigma_j^x \rangle$ and $\langle \tau^z \sigma_i^x \sigma_j^x \rangle$ in the lowest order orthogonality blocking approximation for the case where there is an additional weak bias on the central spin, the results are given in appendix E.3.3. In this case we get a more complicated set of results. We still see quadratic divergences in the various correlators at long times. We will plot these solutions for a specific case in the next chapter. Next we discuss the scaling of the growth rate of larger correlators between the central spin and more bath spins.

Now we consider larger correlators between the central spin and many bath spins. In particular we consider correlators of the form $\langle \tau^\mu \prod_{j \in C} \sigma_j^+ \prod_{j \in K} \sigma_j^- \rangle$ for some subset of the bath $C \subset B$, which are important in the decay of the central qubit polarisation. Because the only terms which contribute to our leading order expansion are those which contain operators which preserve the bath polarisation, at this order the correlator is zero unless $|C|$ is even. Thus it suffices to consider correlators of the form $\langle \tau^\mu \prod_{j \in G} \sigma_j^+ \prod_{j \in K} \sigma_j^- \rangle$, where $G \cup K = C$ and $|G| = |K|$. We have seen the expressions will in general depend on the initial states of the spins in $G$ and $K$, we take $U$ ($D$) to be the subsets of the bath which are initially up (down). Then we will consider the scaling of the correlator

$$\begin{align*}
\langle \tau^\mu \prod_{j \in G} \sigma_j^+ \prod_{j \in K} \sigma_j^- \rangle(t)
&= \text{tr}\left\{U E(t)^\dagger \tau^\mu \prod_{j \in G \cap U} \sigma_j^+ \prod_{j \in K \cap U} \sigma_j^- \prod_{j \in G \cap D} \sigma_j^+ \prod_{j \in K \cap D} \sigma_j^- U E(t) \rho(0)\right\}.
\end{align*}$$

Every spin in $C$ must flip so the leading order expression will have a prefactor of $\prod_{j \in C} \beta_j$. Each bath spin in $C$ will flip alongside one of the central spin flips contained in the transition expansion for either $U E(t)$ or $U E(t)^\dagger$. Those bath spins in $(G \cap U)$ or $(K \cap D)$ must co-flip with one of the central spin flips in the expansion of $U E(t)$. While bath spins in $(G \cap D)$ or $(K \cap U)$ must co-flip with one of the central spin flips in the expansion of $U E(t)^\dagger$. Define the indices $n_L$ and $n_R$,

$$\begin{align*}
n_L &\equiv |G \cap D| + |K \cap U|, \\
n_R &\equiv |G \cap U| + |K \cap D|.
\end{align*}$$

The leading order transition expansion for the correlator (7.90) will then be of the form,

$$\begin{align*}
\langle \tau^\mu \prod_{j \in G} \sigma_j^+ \prod_{j \in K} \sigma_j^- \rangle(t)
&= \left(\prod_{j \in C} \beta_j\right) \Delta_0 t \sum_{m=|n_L-n_R|}^{n_L+n_R} (\Delta_0 t)^m A_{m,c}^\mu \langle \Delta_0 t\rangle.
\end{align*}$$
Where $A_{m,n}^{\mu}(\Delta_0 t)$ is an average over some oscillating term. We see from the expression (7.93), that in the regime of validity of our approximations, correlators involving more bath spins grow slower, while the exact form of the growth depends on the specific correlator.

7.3 Conclusion

In 7.1 we derived a transition expansion for the influence functional for a system of qubits coupled to a spin bath. We have seen that this expansion is most useful when a small number different types of transition are important to understand the dynamics.

Then, in section 7.2 we used this expansion to derive the dynamics of the central spin in the model for precessional decoherence. We saw that the transition Hamiltonian could be simplified by working in basis where the bath spin states depend on the central spin. Then using the approximation of Prokef’ev and Stamp [86] we saw that the important transitions preserved the polarisation group of the bath spin, and we recovered their result for the return probability. Then we showed explicitly (in appendix E.1) how this generalises to give the full central qubit reduced density matrices. We then discussed limitations and corrections to this approximation. We then turned to the build up of correlations between the central qubit and the bath during decoherence. We argued the decoherence in this model via a cascade of correlations, like in the degeneracy blocking model discussed in section 6.1. Except in the precessional decoherence case the information is transferred into correlations with the transverse components of the bath spins, rather than the longitudinal components as seen in degeneracy blocking.

In the next chapter we will apply our results for precessional decoherence, to the Fe$_8$ magnetic molecule qubit.
Chapter 8

Application: The Fe₈ Qubit

As discussed in the section 1.10.2 there are magnetic molecule qubits which possess well understood interactions with their local environment. In this chapter we will explore the dynamics of decoherence in a real magnetic molecule system, the Fe₈ qubit, which is well described by the precessional decoherence Hamiltonian. Examine the results of the previous chapter for the dynamics of the entanglement of the central qubit with its spin environment in the context of this system. In previous work by Stamp, Tupitsyn, and collaborators [73, 98, 101, 103], the relevant parameters have been calculated for the Fe₈ molecule. We will now use these results to calculate the dynamics of the central spin and its correlators with pairs of bath spins in these systems.

8.1 The “Fe₈” Qubit

Here we describe a single such qubit design based on the so called “Fe₈” molecule [40], shown in figure 8.1, the molecule consists of a core of eight Fe³⁺ ions linked by oxo and hydroxo ions and surrounded in a cage of organic ligands. In this section we discuss a qubit made from one of these molecules, ignoring the effect of the environment and in the next section we will discuss its coupling to the environment.

Low temperatures \((T \ll 4K)\), the low energy dynamics of the electronic spins of the Fe³⁺ ions can be described by the following Hamiltonian \(H_{\text{Fe₈}}^0(S)\), written in terms of the total electronic spin \(S\), which is \(S = 10\) [107, 108, 117]

\[
H_{\text{Fe₈}}^0(S) = -DS_z^2 + ES_z^2 + K_4^\perp (S_{\perp}^4 + S_{\perp}^1) - g_e \mu_B \mu_0 S \cdot H_\perp. \tag{8.1}
\]

Here \(H_\perp\) is an applied transverse field (in the \(y\) direction), the energies \(D, E, K_4^\perp\) arise from the details of the molecule, \(g_e\) is the electronic \(g\)-factor, \(\mu_B\) is the Bohr magneton, and \(\mu_0\) is the permeability. Without the applied field, \(S\) feels an anisotropic potential set by the parameters \(D/k_B = 0.23\) K, \(E/k_B = 0.094\) K, \(K_4^\perp = -3.28 \times 10^{-5}\) K [107, 108, 117]. The Hamiltonian (8.1) has been calculated using an ultraviolet high frequency cut-off of \(\Omega_0/k_B = 4.6\) K \((\Omega_0 = 6 \times 10^{11} Hz)\).

The semi-classical potential obtained from the Hamiltonian (8.1) is plotted in figure 8.2 for the experimentally achievable case where the applied transverse field is \(\mu_0 H_\perp = 2.5\) T. From this figure we see there are two minima of energy on the Bloch sphere with opposite \(S_z\) components, states in these two minima can be
Figure 8.1: Structure of the Fe₈ molecule. The crosshatched circles are the Fe³⁺ ions, the hatched circles are the oxygen atoms, and the empty circles represent, in order of decreasing size, nitrogen and carbon atoms. [Reprinted figure with permission, from D Gatteschi, A. Caneschi, L., R. Sessoli, Science, 265, 1054 (1994), [40]. Copyright 1994 by the American Association for the Advancement of Science.].
taken as the two qubit levels, call these states $|⇑\rangle$, and $|⇓\rangle$. These states are strictly defined by

$$|⇑\rangle \equiv \frac{1}{\sqrt{2}} (|s\rangle + |a\rangle)$$  \hspace{1cm} (8.2)

$$|⇓\rangle \equiv \frac{1}{\sqrt{2}} (|s\rangle - |a\rangle),$$  \hspace{1cm} (8.3)

where $|s\rangle$ and $|a\rangle$ are the two lowest energy states of the Hamiltonian (8.1) ($|s\rangle$, and $|a\rangle$ have symmetric and antisymmetric wave functions respectively). From these states one can build the usual Pauli operators ($\tau^z \equiv |⇑\rangle \langle⇑| - |⇓\rangle \langle⇓|$ etc.) and then the effective Hamiltonian for a single isolated Fe$_8$ qubit is of the form [73],

$$H^0_{\text{effFe}_8} = -\frac{1}{2} \Delta_0 (H_\perp) \tau^x.$$  \hspace{1cm} (8.4)

Where $\Delta_0 (H_\perp)$ is as shown in figure [8.3] and has a strong dependence on the applied field. Physically this dependence arises from the fact that as $|H_\perp|$ is increased, the two energy minima move closer to $S_y$ axis (and one another), therefore the tunneling amplitude increases.

### 8.1.1 The Coupling of the Fe$_8$ Qubit to the Spin Bath

At low temperatures, Fe$_8$ is crystalline and the central spin is coupled to an environment primarily consisting of nuclear spins and phonons [85, 98, 101, 103, 118]. The typical time scale $\tau_{\text{ph}}$ associated with the phonon decoherence is [85]

$$\tau_{\text{ph}}^{-1} = \Delta_0^{-1} \left( \frac{4S \Omega_0 \Delta_0}{(k_B \theta_D)^2} \right) ^2 \coth \left( \frac{4\Delta_0}{k_B T} \right).$$  \hspace{1cm} (8.5)

Where $\theta_D$ is the Debye temperature for the crystal, $\theta_D \approx 33K$. So $\tau_{\text{ph}}$ can be made large by using a low field $H_\perp$ to tune $\Delta_0$. $\tau_{\text{ph}}$ is plotted as a function of the applied field in figure [8.4]. This time scale is very long when $H_\perp$ is small, we will see that, at low fields, the spin bath causes much faster decoherence. So we turn to a discussion of the nuclear spin bath.

In terms of the electronic spin operators $s_a$ and the nuclear spin operators $I_j$ the Hamiltonian $H_{\text{Fe}_8\text{SB}}$, which governs the dynamics of the nuclear spins in the Fe$_8$ molecule is of the form,

$$H_{\text{Fe}_8\text{SB}} = \sum_{ja} A^{aj}_{\mu\alpha} s^\mu_a I^\alpha_j + \sum_j g_j^N \mu_j^N \mu_0 H_0 \cdot I_j,$$  \hspace{1cm} (8.6)

where $A^{aj}_{\mu\alpha}$ are the various hyperfine couplings, $H_0$ is the applied magnetic field, $g_j^N$ and $\mu_j^N$ are the g-factor and magnetic moment of the $j$'th nucleus. The precise set of nuclear spins and hyperfine couplings depend on the isotopic make-up of the molecule, but these can be calculated for specific cases [99, 101]. A histogram of the different hyperfine coupling strengths for the $^1$H nuclei and $^{57}$Fe nuclei (for the
Figure 8.2: The energy of the electronic spin vector in the Fe$_8$ molecule. Both the main plot and the inset plot shaded colour shows the semiclassical energy of the electronic spin in the Fe$_8$ molecule as a function of its direction on the Bloch sphere, when the applied field is $\mu_0 H_\perp = 2.5$ T $\hat{y}$. The scale shown on the right gives the energy/$k_B$ in Kelvins. The black bullets (●) mark the positions of the energy minima where the qubit states are localised. The dotted black line marks the semiclassical tunneling route. The inset plot is the same as the main plot but viewed from a different angle.
Figure 8.3: The field dependence of the Fe₈ qubit’s tunneling amplitude $\Delta_0(H_\perp)$, when the field $H_\perp$ is pointing in the $\hat{y}$ direction. Data for this plot is obtained from [73].
Figure 8.4: The time scale associated with decoherence due to phonons in the Fe$_8$ qubit. The field dependence of $\tau_{\text{ph}}$ as a function of the applied field, when the field $\mathbf{H}_\perp$ is pointing in the $\hat{y}$ direction. Data for this plot is obtained from [73], using equation [8.5] and assuming a temperature of $T = 0.5K$. 
Figure 8.5: A histogram of the different hyperfine coupling strengths. The blue boxes show the hyperfine coupling strengths for the H nuclei and the red histogram shows those for $^{57}$Fe nuclei (in the case where all Fe$^{3+}$ ions are $^{57}$Fe). All data is binned into 0.5 MHz intervals. Data for this plot is taken from [99].

case where all the hydrogens in the molecule are $^1H$ and all the iron ions are $^{57}$Fe, both of which are spin $-\frac{1}{2}$) is shown in figure 8.5. A comparison of figures 8.5 and 8.3 shows that if $|H_\perp| \lesssim 1T$ the hyperfine coupling may be quite large compared to the tunneling amplitude.

Now one can proceed truncating the Hamiltonian $H_{Fe_8} = H_{Fe_8}(S) + H_{Fe_8SB}$, to get an effective qubit and spin bath Hamiltonian like (1.48) for the molecule. In this case one finds the $\alpha_i$ terms dressing the qubit flipping term are negligible [98] and one is left with the effective Hamiltonian (neglecting the dipolar interactions between nuclear spins, which can be calculated from the molecular structure and are $\sim 10^{-4} - 0.1$ MHz [99]),

$$H_{eff\ Fe_8} = \frac{\Delta_0(H_0^\perp)}{2}\tau^x + \frac{\tau^z}{2}\sum_i \omega_i^\parallel \sigma_i^z + \frac{1}{2}\sum_i \omega_i^\perp \sigma_i^x.$$  \hspace{1cm} (8.7)

Here $\Delta_0(H_0^\perp)$ is the effective central spin flip amplitude discussed in the previous section, $\omega_i^\parallel$ depends on how much the effective field on the $i$'th nucleus changes when

the central qubit flips,

$$\omega_i^\parallel = \frac{1}{I_i} \left| \sum_a A_{\mu a}^i I^\alpha (\langle s^\mu_a \rangle \uparrow - \langle s^\mu_a \rangle \downarrow) \right|$$  \hspace{1cm} (8.8)

$$\omega_i^\perp = \frac{1}{I_i} \left| \sum_a A_{\mu a}^i I^\alpha (\langle s^\mu_a \rangle \uparrow + \langle s^\mu_a \rangle \downarrow) - g_i^N \mu_i^N \mu_0 H_0^\perp I_i \right|.$$  \hspace{1cm} (8.9)

In the previous two sections we have seen that we can find a well defined effective Hamiltonian for an Fe$_8$ single molecule magnet and its spin bath we will use this in chapter [8] where we study the dynamics of the central spin and the bath in this system.

### 8.2 The Fe$_8$ Molecule in Real Systems

So far experiments on Fe$_8$ magnetic molecules, have been on crystalline samples[41]. This means the qubits in the crystal suffer from some effects which are undesirable for the purpose of this study. Only an ensemble of qubits in the crystal may be addressed experimentally and because of the long ranged dipole fields at play, different qubits can be feeling quite different fields, so we will have to average the results for single over a distribution of different fields. Decoherence also occurs due to the coupling between the average qubit magnetisation in the sample with magnons [73, 103], the decoherence rate due to these interactions, is quite complicated to calculate, and in general depends on the sample geometry. But if one is able to create a small enough crystal the magnon decoherence could be minimised.

### 8.3 Dynamics of Dechoerence Due to $^1$H Nuclei

We are interested in the details of the loss of information in the central qubit and how correlations build up with the bath spins. As we saw in the previous chapter the relevant parameter determining for the “strength” of the spin bath is $\kappa$. The most important nuclei for the spin decoherence at low fields (where the effect of phonons is small), are the $^1$H nuclei [99]. This $\kappa$ parameter has been calculated [99] from the various $^1$H couplings and is shown in figure [8.6] as a function of field strength $H_\perp$.

We now consider a definite case, when the applied field is $\mu_0 H_\perp = (0.025 \text{ T}) \hat{y}$, then the tunneling element is $\Delta_0 \approx 2.47 \times 10^4 \text{ Hz}$. First we give results for a hypothetical experiment where we prepare a single Fe$_8$ qubit, so that the bath of $^1$H nuclei is in a definite state in the zero polarisation group and we have tuned the $z$ component of the magnetic field so the central qubit experiences no bias. If
Figure 8.6: A plot of the variable $\kappa$ parametrising the bath of $^1$H nuclei in the Fe$_8$.

The plotted data is obtained from [99] and it corresponds to the case where all of the hydrogen atoms in the molecule are $^1$H.

then the central system is prepared so that it is fully polarised in the $z$ direction, we are be able to use the results of the previous section and the time evolution of the central spin is as given in figure [8.7] The results we would obtain were we able to measure the time dependence of correlators between the central spins given in equations (7.75-7.81) or (7.82-7.89), (depending on the initial states of the specific bath spins) are also shown in figure [8.7].

We see that correlator $\langle \sigma_i^x \sigma_i^x \rangle$ increases and amplitude amplitude of correlators like $\langle \tau_z \sigma_i^x \sigma_i^x \rangle$ increase as the central qubit loses information to the bath. If we were not able to measure these correlators for specific pairs of bath spins, but instead we had to measure the average of these correlators over all choices for pairs of bath spins then the only correlators with pairs of off diagonal bath components, which would not average out to zero, would be $\langle \tau_z \sigma_i^x \sigma_j^x \rangle = \langle \tau_z \sigma_i^y \sigma_j^y \rangle$ and $\langle \tau_z \sigma_i^x \sigma_j^x \rangle$ and they would be as shown in figure [8.8]. In this case we would still see the growth of the important correlators as the central spin loses information.

Unfortunately such experiments on a single Fe$_8$ molecule have not yet been achieved. Experiments have been done on crystals of Fe$_8$, but in these samples the individual molecules feel a range of biases $\delta \xi$, which has been measured $\delta \xi \sim 5 \times 10^7$ Hz [103], which will completely wash out the details of the dynamics seen here. Even if a single molecule could be isolated and experimented on the range of different couplings due to the dipolar hyperfine coupling between the $^1$H molecules is quite
Figure 8.7: Plots of the correlators for the case of a single Fe$_8$ molecule coupled to its $^1$H nuclear spin bath, as described in section 8.3. The top graph shows the time dependence of the components of the central spin polarisation, $\langle \pi \rangle$, the solid red curve is $\langle \pi^x \rangle$, the dashed green curve is $\langle \pi^y \rangle$, and the dotted blue curve is $\langle \pi^z \rangle$. The bottom left graph shows components of correlators involving two bath spins, $i$ and $j$, where spin $i$ is initialy up and $j$ is initialy down. The bottom right graph shows components of the same correlators (when they are non-zero) in the case that spins $i$ and $j$ are intialy aligned. In the main plots on the bottom, the dotted blue curve is $\langle \pi^z \sigma^x_i \sigma^x_j \rangle = \langle \pi^z \sigma^y_i \sigma^y_j \rangle$, the dashed green curve is $\langle \pi^y \sigma^x_i \sigma^x_j \rangle$, the solid red curve is $\langle \pi^y \sigma^x_i \sigma^y_j \rangle = \langle \pi^y \sigma^y_i \sigma^x_j \rangle$, and in the inset the thick solid red curve is $\langle \pi^x \sigma^x_i \sigma^x_j \rangle$, the dashed red curve is $\langle \pi^x \sigma^y_i \sigma^x_j \rangle$, and the thin black curve is $\langle \sigma^x_i \sigma^x_j \rangle$. 
Figure 8.8: A plot of correlators between the bath spins and the central spin, for the case of a single Fe₈ molecule coupled to its ¹H nuclear spin bath, when we have averaged over the different choices for sites i and j. The dotted blue curve is \( \langle \tau_z \sigma_x^i \sigma_x^j \rangle = \langle \tau_z \sigma_y^i \sigma_y^j \rangle \) and the dashed green curve is \( \langle \tau_y \sigma_x^i \sigma_x^j \rangle \).

large, we estimate \( \delta \omega \sim 2 \times 10^5 \text{ Hz} \) (from data in [99]), which will have a similar effect destroying the results we see here. As such in the next section we will consider a molecule where all of the hydrogen atoms are substituted by deuterium, and the decoherence is caused by the other nuclei.

8.4 Dynamics of Decoherence Due to \(^{57}\text{Fe}\) Nuclei

We saw in the previous section that a realistic test of the precessional decoherence model due to the ¹H spin bath is unfeasible, even on a single molecule, due to the spread of different couplings between the hydrogen nuclei and the central qubit. We saw in section 8.1.1 that in the case where the Fe³⁺ ions are the \(^{57}\text{Fe}\) isotope, then the spread of the distribution of the contact hyperfine couplings between these ions and the electronic spins is smaller. We calculate \( \delta \omega \sim 2 \times 10^5 \text{ Hz} \) (from data in [99]), which is much smaller, than that associated with the hydrogen. Also with the hydrogen spin bath eliminated by isotopic substitution, the coherence time will be longer and higher a field \( \mathbf{H}_\perp \) can be used resulting in a bigger \( \Delta_0 \), so the dimensionless ratio \( \delta \omega / \Delta_0 \) can be made much smaller.

We consider a case where all the nuclei except the iron nuclei are spin zero isotopes and all the iron nuclei are \(^{57}\text{Fe}\). If the applied field is \( \mathbf{H}_\perp = 1 \text{ T} \), then we have a transition amplitude \( \Delta_0 = 81.0 \text{ MHz} \) (see figure [8.3], at \( T = 0.5K \)) and the timescale associated with phonon decoherence is \( \tau_{ph} = 25 \text{ s} \) (from equation (8.5), at \( T = 0.5K \)). By assuming the contact hyperfine interaction between the nuclear spins and the electronic spins is isotropic, we can calculate the \( \beta_i \approx 0.05 \) and \( \kappa \approx 0.01 \) using equations (8.8) and (8.8). Then we plot results for the central
spin polarisation, and the non-zero correlators with pairs of bath spins in figure 8.9 for the initial period of decoherence. In these results we have averaged the results in appendix E.3.3, for precessional decoherence with a small bias, over a Gaussian distribution of biases with standard deviation $\delta \omega$. This average should account for experiments either perform an ensemble of different measurements, or study an ensemble of different systems with slightly different biases. We also assume we can not probe particular pairs iron nuclei, so we have averaged over the different choices for bath spins $i$ and $j$. We see that as the central qubit decays correlations build up with pairs of bath spins.

8.5 Conclusion

The important result of this section is that, if one can perform measurements on a single Fe$_8$ molecule, in which all the nuclei are isotopes with spin zero, except the iron ions which are the $^{57}$Fe isotope, then we can predict the correlators of components of the central spin with the transverse components of pairs of bath spins. We think these could be measured using NMR techniques, the details of such an experiment are left for future work.
Figure 8.9: The initial stages of decoherence in an Fe₈ qubit, when we have averaged over the different choices for bath spins $i$ and $j$. The top figure shows components of the central qubit $\langle \tau \rangle$, the solid red curve is $\langle \tau^x \rangle$, the dashed green curve is $\langle \tau^y \rangle$, and the dotted blue curve is $\langle \tau^z \rangle$. The bottom figure is plot of correlators between the pairs of bath spins and the central spin, the dotted blue curve is $\langle \tau^z \sigma^x_i \sigma^x_j \rangle = \langle \tau^y \sigma^y_i \sigma^y_j \rangle$ and the dashed green curve is $\langle \tau^y \sigma^y_i \sigma^y_j \rangle$. 
Chapter 9

Evolution of a Large “Cat State”

Here we will consider the time evolution of a set $\mathcal{S}$ containing $N$ central spins where the initial state is a “cat-state”. These states have a wave function which is a coherent superposition of two states where all the spins have opposite components in the $z$ (quantisation) direction. We can specify these states in terms of the ket $|s\rangle$ with a vector $s = (s_1, s_2, \ldots, s_N)$ where each element $s_a = \pm 1$ indicates whether the $a$’th spin in $\mathcal{S}$ is up or down and $|s\rangle = \prod_{a \in \mathcal{S}} |s_a\rangle$. We consider initial states that can be described by the wave function,

$$|\psi_{s,\phi}\rangle = \frac{1}{\sqrt{2}} \left( |s\rangle + e^{i\phi} |\bar{s}\rangle \right), \quad (9.1)$$

where we have allowed for an arbitrary phase angle $\phi$ between the two parts of the superposition.

The initial reduced density matrix for $\mathcal{S}$ (we allow for the possibility that $\mathcal{S}$ is part of a large set of qubits the others forming an environment) is then

$$\bar{\rho}_S(0) = \frac{1}{2} \left( |s\rangle\langle s| + |\bar{s}\rangle\langle\bar{s}| + e^{i\phi} |\bar{s}\rangle\langle s| + e^{-i\phi} |s\rangle\langle\bar{s}| \right). \quad (9.2)$$

In the following sections we will discuss the specifics of the time evolution of these cat states in a variety of cases. First in section 9.1 we will discuss some quantities which will be useful to characterise the information contained in the reduced density matrix $\bar{\rho}_S(t)$ as time evolves. In section 9.2 we consider the case where each spin only feels the its own longitudinal field in that case the phase angle the evolution is equivalent to the phase angle $\phi$ evolving with time at a frequency determined by the vector $s$. In section 9.3 we study the case where each spin feels a general local field and find that when the fields have a transverse component for large $N$ many of the quantities we are interested are zero most of the time except at given recurrence times determined by the mean strength of the field and that the effect of these local fields being disordered is to modulate these recurrences by a function that decays on a time scale determined by the spread of the frequencies. In section 9.4 we discuss the case where each spin interacts with its own static environment so that the field each spin feels is effectively averaged over a range of values, we find that there are several regimes for the decay of the recurrences seen in this model in various
quantities and that the importance of these regimes is determined by how large
$N$ is. In section 9.5 we will consider the case where the effect of the environment
causes more general averaging of the central spin dynamics and elucidate which of
the results in the degeneracy blocking case can be generalised.

9.1 Quantities of Interest

We will assume that the system $S$ and the environmental bath $B$ are initially in
a product state $\rho(0) = \rho_S(0)\rho_B(0)$. First we can split the initial reduced density
matrix $\bar{\rho}_S(0) = \hat{D}(0) + \hat{C}(0)$ into a diagonal $\hat{D}(0)$ and off diagonal parts $\hat{C}(0)$,

$$\hat{D}(0) = \frac{1}{2} \left( |s\rangle\langle s| + |s\rangle\langle -s| \right) = \frac{1}{2N+1} \prod_{a \in S} (1 + s_a\tau_a^z) + \frac{1}{2N+1} \prod_{a \in S} (1 - s_a\tau_a^z) \quad (9.3)$$

$$\hat{C}(0) = \frac{1}{2} \left( e^{i\phi}|s\rangle\langle -s| + e^{-i\phi}|s\rangle\langle -s| \right) = \frac{1}{2} \left( \frac{e^{i\phi}}{2N} \prod_{a \in S} (\tau_a^x - i s_a\tau_a^y) + \text{h.c.} \right). \quad (9.4)$$

Where h.c. denotes the Hermitian conjugate of the previous term. From the expres-
sions (9.3) and (9.4) we can describe all correlations which specify the initial state.
The diagonal part (9.3) contains correlators between $z$ components of the spins only.
$\hat{D}(0)$ is a valid (impure) density matrix on its own and would describe state which
could be described by classical a probability distribution where for the out come of
the $z$ component vector $\tilde{s}$ occurs with probability $P_{\tilde{s}} = \frac{1}{2} \left( \delta_{\tilde{s},s} + \delta_{\tilde{s},-s} \right)$. A correlator
between the $z$ components of a cluster $C \subseteq S$ of the spins is only non-zero when the
cluster contains an even number of spins ($|C|$ is even) in which case it is

$$\left\langle \prod_{a \in C} \tau_a^z(0) \right\rangle = \prod_{a \in C} s_a. \quad (9.5)$$

The off diagonal part (9.3) contains only correlators between $x$ and $y$ components
of spins furthermore it contains only correlators containing all $N$ qubits, no smaller
clusters. This means that if any spin is traced out of $\bar{\rho}_S(0)$ then all the off-diagonal
information is lost and there are no non-zero correlators involving $\tau_a^x$ or $\tau_a^y$ in the
resulting density matrix, so we see that $\hat{C}(0)$ contains information about the $N$-
partite quantum entanglement of the state. Now as the density matrix evolves
with time we can define time dependent operators $D(t) = \text{tr}_B U(t)\hat{D}(0)\rho_B(0)U^\dagger(t)$
and $\hat{C}(t) = \text{tr}_B U(t)\hat{C}(0)\rho_B(0)U^\dagger(t)$ which give us the parts of the density matrix
$\bar{\rho}_S(t) = \text{tr}_B U(t)\rho(0)U^\dagger(t) = \hat{D}(t) + \hat{C}(t)$ sourced by the initial diagonal and off
diagonal parts respectively. In general $\hat{D}(t)$ and $\hat{C}(t)$ will contribute to all possible
correlators at finite times and we can expand them in terms of these contributions,

\[ \hat{D}(t) = \frac{1}{2N} \sum_{C \subseteq S} D_{\mu_1, \ldots, \mu_{|C|}}(t) \prod_{a_i \in C} \tau^{\mu_a}_{a_i} \]  \hspace{1cm} (9.6) \\
\hat{C}(t) = \frac{1}{2N} \sum_{C \subseteq S} C_{\mu_1, \ldots, \mu_{|C|}}(t) \prod_{a_i \in C} \tau^{\mu_a}_{a_i} \]  \hspace{1cm} (9.7) \\
with : 

\[ D_{\mu_1, \ldots, \mu_{|C|}}(t) = \text{tr}_S \hat{D}(t) \prod_{a_i \in C} \tau^{\mu_a}_{a_i} \]  \hspace{1cm} (9.8) \\
\[ C_{\mu_1, \ldots, \mu_{|C|}}(t) = \text{tr}_S \hat{C}(t) \prod_{a_i \in C} \tau^{\mu_a}_{a_i}. \]  \hspace{1cm} (9.9)

Note that the above implies \( D^{\emptyset}(t) = 1, C^{\emptyset}(t) = 0 \) and that a correlator between a cluster \( C \) of spins has a contribution from both \( \hat{D}(t) \) and \( \hat{C}(t) \),

\[ \left\langle \prod_{a \in C} \tau^{\mu_a}_{a}(t) \right\rangle = D_{\mu_1, \ldots, \mu_{|C|}}(t) + C_{\mu_1, \ldots, \mu_{|C|}}(t). \]  \hspace{1cm} (9.11)

One could imagine an experiment to measure the components of the tensors \{\( C_{\mu_1, \ldots, \mu_{|C|}}(t), D_{\mu_1, \ldots, \mu_{|C|}}(t) \}\) suppose one has the means to prepare two copies of central system, (a) in the cat state (9.2) but also (b) in the impure state where \( \rho_S(0) = \hat{D}(0) \) then one could measure the correlator \( \left\langle \prod_{a \in C} \tau^{\mu_a}_{a}(t) \right\rangle \) in both systems after some time then one has

\[ D_{\mu_1, \ldots, \mu_{|C|}}(t) = \left\langle \prod_{a \in C} \tau^{\mu_a}_{a}(t) \right\rangle \]  \hspace{1cm} (a) and \[ C_{\mu_1, \ldots, \mu_{|C|}}(t) = \left\langle \prod_{a \in C} \tau^{\mu_a}_{a}(t) \right\rangle \]  \hspace{1cm} (b).

Initially when the central spins are in a cat state the tensors \( \{C^C, D^C\} \) are

\[ C_{\mu_1, \ldots, \mu_{|C|}}(0) = \delta_{C S} \Re e^{i\phi} \prod_{a \in S} (\hat{x}_{\mu_a} - i\hat{y}_a) \]  \hspace{1cm} (9.12) \\
\[ D_{\mu_1, \ldots, \mu_{|C|}}(0) = \begin{cases} 
\prod_{a \in C} s_a \hat{z}_{\mu_a} & \text{for } |C| \text{ even} \\
0 & \text{for } |C| \text{ odd}.
\end{cases} \]  \hspace{1cm} (9.13)

One quantity of interest is the probability \( p_r(t) \) for the state at \( t \) to return to its initial state. When written in terms of the operators \( \hat{C} \) and \( \hat{D} \) the return probability is

\[ p_r(t) = \text{tr} S \tilde{\rho}_S(t) \tilde{\rho}_S(0) = \text{tr}_S \hat{D}(t) \hat{D}(0) + \text{tr}_S \hat{D}(t) \hat{C}(0) + \text{tr}_S \hat{C}(t) \hat{D}(0) + \text{tr}_S \hat{C}(t) \hat{C}(0) \]  \hspace{1cm} (9.14) \\
the last term \( \text{tr}_S \hat{C}(t) \hat{C}(0) \) is of particular interest because it tells us how much of the off-diagonal part of the density matrix returns to its original value we will refer to this as the off-diagonal part of the return probability \( p_c(t) \)

\[ p_c(t) \equiv \text{tr}_S \hat{C}(t) \hat{C}(0). \]  \hspace{1cm} (9.15)
Note that $p_c(t)$ is not a valid probability as it may be negative so it is probably best thought of as the inner-product of $\hat{C}(t)$ with its initial value. We can write the terms appearing in the above expression in terms of the tensors $\{D^C_{\mu_1...}(t), C^C_{\mu_1...}(t)\}$,

\[
\text{tr}_S \hat{D}(t) \hat{D}(0) = \sum_{\substack{\mathcal{C} \subseteq S \, |\mathcal{C}| \text{ even}}} \frac{1}{2^N} D^C_{zz...z}(t) \prod_{a \in \mathcal{C}} s_a
\]

(9.16)

\[
\text{tr}_S \hat{C}(t) \hat{D}(0) = \sum_{\substack{\mathcal{C} \subseteq S \, |\mathcal{C}| \text{ even}}} \frac{1}{2^N} C^C_{zz...z}(t) \prod_{a \in \mathcal{C}} s_a
\]

(9.17)

\[
\text{tr}_S \hat{D}(t) \hat{C}(0) = \text{Re} \frac{e^{i\phi}}{2^N} D^S_{\mu_1...\mu_N}(t) \prod_{a \in S} (\hat{x}^{\mu_a} - i s_a \hat{y}^{\mu_a})
\]

(9.18)

\[
\text{tr}_C \hat{D}(t) \hat{C}(0) = \text{Re} \frac{e^{i\phi}}{2^N} C^S_{\mu_1...\mu_N}(t) \prod_{a \in S} (\hat{x}^{\mu_a} - i s_a \hat{y}^{\mu_a}).
\]

(9.19)

Also note the return probability can be written directly in terms of the correlators at the initial and final times

\[
p_r(t) = \sum_{\mathcal{C} \subseteq S} \frac{1}{2^N} \left< \prod_{a \in \mathcal{C}} \tau^{\mu_a}_a(t) \right> \left< \prod_{a \in \mathcal{C}} \tau^{\mu_a}_a(0) \right>.
\]

(9.20)

The return probability diagnoses how likely the system is to return to its initial state. In general a large isolated system could take an effectively infinite amount of time to have a good probability of returning to its initial state thus we could expect $p_r(t)$ and related metrics to decay on time scales less than this recurrence time even though no information would be lost to an environment. A quantity that tells us about information loss to the environment is the trace of the reduced density matrix squared

\[
p(t) \equiv \text{tr}_S \bar{\rho}_S(t)^2
\]

(9.21)

which is sometimes called the purity[78] and is related to the linear entropy discussed in section[1.4.1]. The purity is one for a pure state and $\frac{1}{2^N} \leq p < 1$ for a mixed state. The purity can be expressed in terms of $\hat{C}(t)$ and $\hat{D}(t)$

\[
p(t) \equiv \text{tr}_S \bar{\rho}_S(t)^2 = \text{tr}_S \hat{D}(t) \hat{D}(0) + 2 \text{tr}_S \hat{C}(t) \hat{D}(t) + \text{tr}_S \hat{C}(t) \hat{C}(t).
\]

(9.22)

Note that expressions like $\text{tr}_S \hat{C}(t) \hat{D}(t)$ can be written in terms of the tensor components for example

\[
\text{tr}_S \hat{C}(t) \hat{D}(t) = \sum_{\mathcal{C} \subseteq S} \frac{1}{2^N} C^C_{\mu_1...\mu_{|\mathcal{C}|}}(t) D^C_{\mu_1...\mu_{|\mathcal{C}|}}(t).
\]

(9.23)
If our central system is isolated then the purity is constant and we have the following

\[ \text{tr}_S \hat{D}(t)\hat{D}(t) = \text{tr}_S U(t)\hat{D}(0)U^\dagger(t)\hat{D}(0)U^\dagger(t) = \frac{1}{4} \text{tr}_S (|s\rangle \langle s| + | - s\rangle \langle - s|) = \frac{1}{2} \]  

(9.24)

\[ \text{tr}_S \hat{C}(t)\hat{D}(t) = 0 \]  

(9.25)

\[ \text{tr}_S \hat{C}(t)\hat{C}(t) = \frac{1}{2} \]  

(9.26)

so that the purity can be divided into equal parts belonging to the diagonal and off-diagonal parts which are constant over time. The purity can also be expanded in terms of correlators

\[ p(t) = \frac{1}{2N} \sum_{\mathcal{C} \subseteq \mathcal{S}} \left( \prod_{a \in \mathcal{C}} \tau^x_a(t) \right) \left( \prod_{b \in \mathcal{S} \setminus \mathcal{C}} \tau^y_b(t) \right) \equiv \sum_{\mathcal{C} \subseteq \mathcal{S}} p_\mathcal{C}(t). \]  

(9.27)

There are contributions to the purity from each of the correlators, of particular interest is \( p_\mathcal{S} \) which describes the contribution to the purity from the \( N \)th order correlators. We can get an understanding of the entanglement properties by looking at the correlators. Of particular interest is the off-diagonal \( N \) point correlators for the central system that is the correlators of the form \( \langle \prod_{a \in \mathcal{C}} \tau^x_a(0) \prod_{b \in \mathcal{S} \setminus \mathcal{C}} \tau^y_b(0) \rangle \) where \( \mathcal{C} \subseteq \mathcal{S} \). Really we should look at the irreducible version of this correlator (initially the irreducible correlator is identical to the correlator). Initially the \( N \) point correlators in the \( x-y \) plane are,

\[ \left\langle \prod_{a \in \mathcal{C}} \tau^x_a(0) \prod_{b \in \mathcal{S} \setminus \mathcal{C}} \tau^y_b(0) \right\rangle = \cos \left( \phi - \frac{\pi |\mathcal{C}|}{2} \right). \]  

(9.28)

We can get an idea of how much information is contained in these correlators by looking at the contribution to the purity from these correlators alone,

\[ p_{\perp \mathcal{S}}(t) = \frac{1}{2N} \sum_{\mathcal{C} \subseteq \mathcal{S}} \left( \prod_{a \in \mathcal{C}} \tau^x_a \right) \left( \prod_{b \in \mathcal{S} \setminus \mathcal{C}} \tau^y_b \right)^2 \]  

(9.29)

initially \( p_{\perp \mathcal{S}}(0) = \frac{1}{2} \) (so it contains the entire purity of the off-diagonal part of the density matrix). As time goes by \( p_{\perp \mathcal{S}} \) may be lost to the environment or other correlators in the system. An alternate formula \( p_{\perp \mathcal{S}}(t) \) which may be simpler to calculate is

\[ p_{\perp \mathcal{S}}(t) = \frac{1}{2N} \left\langle \tau^{\mu_1}_{\nu_1} \cdots \tau^{\mu_N}_{\nu_N} \right\rangle \prod_{\mu \nu} \mathbb{P}^-_{\mu \nu} \left\langle \tau^{\nu_1}_{\mu_1} \cdots \tau^{\nu_N}_{\mu_N} \right\rangle \]  

(9.30)

where \( \mathbb{P}^-_{\mu \nu} = \delta_{\mu \nu} - \hat{z}_\mu \hat{z}_\nu \) is the projection operator that projects every polarisation into the \( x-y \) plane.
9.2 Motion in Applied Longitudinal Fields

The first case we will consider is where the central Hamiltonian contains a local longitudinal field for each central spin and there is no interaction with the bath so that the central system is isolated with a Hamiltonian

$$H = \frac{1}{2} \sum_a \xi_a \tau_a^z.$$ (9.31)

The off diagonal part of $\rho$ evolves

$$\dot{\hat{C}}(t) = \frac{1}{2} U(t)(e^{-i\phi} |s\rangle\langle -s| + e^{i\phi} |s\rangle\langle -s|) U\dagger(t)$$ (9.32)

$$= \frac{1}{2} (e^{-i\phi - \sum_a s_a \xi_a t} |s\rangle\langle -s| + e^{i\phi + \sum_a s_a \xi_a t} |s\rangle\langle -s|).$$ (9.33)

Thus the Hamiltonian effectively causes the phase $\phi$ to accumulate over time. Thus the contribution from the off diagonal part to the return probability oscillates with time and does not decay

$$\text{tr} \hat{C}(t) \hat{C}(0) = \cos \left( \phi + \sum_a s_a \xi_a t \right).$$ (9.34)

The diagonal part of the density matrix commutes with the Hamiltonian and is conserved. The return probability in this case is then

$$p_r(t) = \text{tr} \rho(t) \rho(0) = \frac{1}{2} \left( 1 + \text{tr} \hat{C}(t) \hat{C}(0) \right).$$ (9.35)

Only the off-diagonal correlators have a time dependence and because there are only local fields. A correlator on set $C$ only depends on correlators containing all the spins from that set initially so that the only non-zero off diagonal correlators are those encompassing the whole system, so for an arbitrary subset $C \subseteq S$ we have

$$\left\langle \prod_{a \in S \setminus C} \tau_a^x(t) \prod_{b \in C} \tau_b^y(t) \right\rangle = \cos \left( \phi + \sum_{c \in S} s_c \xi_c t + \frac{\pi}{2} |C| \right).$$ (9.36)

All of the off diagonal correlators oscillate at the same frequency as the return probability. As the Hamiltonian (9.31) contains no coupling to the environment the off diagonal and diagonal purities are conserved and the off diagonal part of $\hat{C}(t)$ remains off diagonal, so the purity contained in the $N$ order off diagonal correlators is $p_{\perp S}(t) = \text{tr} \hat{C}(t)^2 = \frac{1}{2}$ constant. Intuitively we can understand this evolution as all of the components contained in the correlators freely rotating around the $\hat{z}$ axis, only the $N$’th order correlators have any components in the $x-y$ plane so only they evolve but their magnitude remains the same.
9.3 Motion in General fields

Consider the case where the Hamiltonian consists of local fields for every site which are each individually at an angle $\theta_a$ to the axis of quantisation and have strength $\omega_a$

$$H = \frac{1}{2} \sum_a \omega_a (\cos \theta_a \hat{\mathbf{x}} + \sin \theta_a \hat{\mathbf{z}}) \cdot \tau_a = \sum_a (\Delta_a \hat{\mathbf{x}} + \xi_a \hat{\mathbf{z}}) \cdot \tau_a. \quad (9.37)$$

Because the Hamiltonian is local the different order correlators evolve independently and so that the only tensor components of $\hat{C}(t)$ that is non-zero are those contained in $C_{\mu_1...\mu_N}^S$ (i.e. those containing components of all the spins) which we will abbreviate as $C_{\mu_1...\mu_N}$ in this section. At time $t$ we have

$$C_{\mu_1...\mu_N}(t) = \frac{1}{2} \text{Re} e^{i\phi} \prod_a (g_{a}^{\mu_\alpha^x}(t) - is_a g_{a}^{\mu_\alpha^y}(t)). \quad (9.38)$$

Where $g_{a}^{\mu_\nu}(t)$ is the single spin Green function (cf.(4.24)) for the qubit $a$

$$g_{a}^{\mu_\nu}(t) = \hat{h}_a^{\mu} \hat{h}_a^{\nu} + \cos(\omega_a t) \left( \delta^{\mu_\nu} - \hat{h}_a^{\mu} \hat{h}_a^{\nu} \right) + \sin(\omega_a t) \varepsilon^{\mu_\nu_\lambda} \hat{h}_a^{\lambda} \quad (9.39)$$

where $\hat{h} = \cos \theta_a \hat{\mathbf{z}} + \sin \theta_a \hat{\mathbf{x}}$ is the direction of the field on spin $a$. Thus the off-diagonal contribution to the return probability is

$$\text{tr} \hat{C}(t) \hat{C}_0 = \frac{1}{2} \text{Re} \left\{ e^{2i\phi} \prod_a \left[ \frac{1}{2} \cos^2 \theta_a (1 - \cos \omega_a t) \right. \right.$$

$$\left. + \prod_a \left[ \frac{1}{2} \cos^2 \theta_a + (2 - \cos^2 \theta_a) \cos \omega_a t + 2i \sin \theta_a \sin \omega_a t \right] \right. \right.$$

$$\left. + \prod_{a \in K} \left[ \frac{1}{2} \cos^2 \theta_a + (2 - \cos^2 \theta_a) \cos \omega_a t - 2i \sin \theta_a \sin \omega_a t \right] \right. \right.$$
is the same so that $\theta_a = \theta_0$ and $\omega_a = \omega_0$ in which case

$$\text{tr} \hat{C}(t)\hat{C}_0 = \frac{1}{2} \text{Re} \left\{ e^{2i\phi} \left[ \frac{1}{2} \cos^2 \theta_0(1 - \cos \omega_0 t) \right]^N + \frac{1}{2} \left[ \cos^2 \theta_0 + (2 - \cos^2 \theta_0) \cos \omega_0 t - 2i \sin \theta_0 \sin \omega_0 t \right]^N \right\}. \quad (9.42)$$

Each of the terms inside the curly brackets is proportional to some number which is less than one raised to a large power $N$ as such they are exponentially small in $N$ unless the number has a magnitude close to one. So terms are not exponentially small in $N$ when,

$$\left| \frac{1}{2} \cos^2 \theta_0(1 - \cos \omega_0 t) \right| = 1 \Rightarrow \theta_0 = \pi n \text{ and } \omega_0 t = \pi(2m + 1) \quad (9.43)$$

$$\frac{1}{2} \left| \cos^2 \theta_0 + (2 - \cos^2 \theta_0) \cos \omega_0 t - 2i \sin \theta_0 \sin \omega_0 t \right| = 1 \Rightarrow \omega_0 t = 2\pi \ell \text{ or } \theta_0 = \frac{\pi}{2}(2k + 1) \quad (9.44)$$

for $n,m,\ell,k \in \mathbb{Z}$. We can expand around these points to get the large $N$ asymptotic behaviour at these points, for instance let $\omega_0 t = \pi + \omega_0 \delta t$ and $\theta_0 = \pi + \delta \theta_0$ then for small $\delta t$ and $\delta \theta_0$

$$\left[ \frac{1}{2} \cos^2 \theta_0(1 - \cos \omega_0 t) \right]^N \sim e^{-N\delta \theta_0^2 - \frac{1}{4}N(\omega_0 \delta t)^2} \quad (9.45)$$

replacing the small terms with trigonometric approximations with the correct periodicity gives,

$$\left[ \frac{1}{2} \cos^2 \theta_0(1 - \cos \omega_0 t) \right]^N \sim e^{-N \sin^2 \theta_0 - N \cos^2 \left( \frac{\omega_0 t}{2} \right)} \quad (9.46)$$

Similarly near $t = 2\pi/\omega_0 \ell$ for $\ell \in \mathbb{Z}$ the magnitude of the second product in $(9.42)$ is

$$\frac{1}{2^2} \left| \cos^2 \theta_0 + (2 - \cos^2 \theta_0) \cos \omega_0 t - 2i \sin \theta_0 \sin \omega_0 t \right|^N \sim e^{-N \frac{\cos^2(\theta_0)\omega_0^2}{4} \left( t - \frac{2\pi}{\omega_0} \right)^2} \quad (9.47)$$

so the product will be $e^{-N \frac{\cos^2(\theta_0)\omega_0^2}{4} \left( t - \frac{2\pi}{\omega_0} \right)^2} e^{i\Phi(t)}$ where $\Phi(t)$ is the phase angle close to each of the $t = 2\pi/\omega_0 \ell$ we find

$$\Phi(t) \sim -N \omega_0 \sin \theta_0 \left( t - \frac{2\pi}{\omega_0} \ell \right) = -N \xi_0 \left( t - \frac{2\pi}{\omega_0} \ell \right). \quad (9.48)$$
So that as $N \to \infty$

\[
\frac{1}{2^N} \left[ \cos^2 \theta_0 + (2 - \cos^2 \theta_0) \cos \omega_0 t - 2i \sin \theta_0 \sin \omega_0 t \right]^N \sim \sum_{\ell=0}^{\infty} e^{-\frac{N}{4} \omega_0^2 \cos^2(\theta_0) \left( t - \frac{2\pi \ell}{\omega_0} \right)^2 - iN \xi_0 \left( t - \frac{2\pi \ell}{\omega_0} \right)}
\]  

(9.49)

or equivalently

\[
\frac{1}{2^N} \left[ \cos^2 \theta_0 + (2 - \cos^2 \theta_0) \cos \omega_0 t - 2i \sin \theta_0 \sin \omega_0 t \right]^N \sim e^{-N \cos^2 \theta_0 \sin^2(\frac{\omega_0 t}{2})} - iN \xi_0 t + i\vartheta(t)
\]  

(9.50)

here $\vartheta(t)$ is a slowly varying function of time that ensures the phase is zero when ever $t = 2\pi \ell/\omega_0$. So that for large $N$ we have the off-diagonal part of the return probability

\[
p_c(t) = \text{tr} \hat{C}(t) \hat{C}_0 \sim \frac{1}{2} \cos(2\phi) e^{-N \sin^2 \theta_0 - N \cos^2(\frac{\omega_0 t}{2})}
\]  

(9.51)

\[
+ \frac{1}{2} \cos(N \xi_0 t + \vartheta(t)) e^{-N \cos^2 \theta_0 \sin^2(\frac{\omega_0 t}{2})}.
\]

Now consider the case where $N$ is even and the effect of the diagonal part of the initial density matrix, we have (when all $s_a = +1$)

\[
D^S_{\mu_1...\mu_N}(t) = \prod_a g^{\mu_a\bar{\mu}_a}(t).
\]  

(9.52)

So the contribution to the return probability from the diagonal $N$ point correlator alone is

\[
\frac{1}{2^N} D^S_{\mu_1...\mu_N}(t) D^S_{\mu_1...\mu_N}(0) = \frac{1}{2^N} \prod_a g^{zz}(t)
\]  

(9.53)

\[
= \frac{1}{2^N} \prod_a \left[ \sin^2 \theta_a + \cos \omega_a t (1 - \sin^2 \theta_a) \right]
\]  

(9.54)

all terms in the product (9.54) are less than $\frac{1}{2}$ so this is exponentially small for large $N$ compared to $\text{tr} \hat{C}(t) \hat{C}_0$. Similarly the cross terms which contribute to the return probability,

\[
\text{tr} \hat{D} \hat{C}_0 = \frac{1}{2^N} \text{Re} e^{i\phi} \prod_a \cos \theta_a [\sin \theta_a (1 - \cos \omega_a t) - i \sin \omega_a t]
\]  

(9.55)

\[
\text{tr} \hat{C} \hat{D}_0 = \frac{1}{2^N} \text{Re} e^{i\phi} \prod_a \cos \theta_a [\sin \theta_a (1 - \cos \omega_a t) + i \sin \omega_a t]
\]  

(9.56)
are exponentially small as well. So we see that the leading order contribution from the \(N\) point correlators to the return probability is \((9.51)\). The total diagonal part of the return probability is

\[
\text{tr} \hat{D}(t) \hat{D}(0) = \frac{1}{4} \text{tr} \left( U(t) |\hat{g}\rangle \langle \hat{g}| U^\dagger(t) |\hat{g}\rangle \langle \hat{g}| + U(t) |\hat{g}\rangle \langle \hat{g}| - |\hat{g}\rangle \langle \hat{g}| - U(t) |\hat{g}\rangle \langle \hat{g}| U^\dagger(t) |\hat{g}\rangle \langle \hat{g}| \right) \quad (9.57)
\]

\[
= \frac{1}{2} \prod_{a \in \mathcal{S}} \left( \frac{1 + s_ag_{a}^{zz}(t)}{2} \right) + \frac{1}{2} \prod_{a \in \mathcal{S}} \left( \frac{1 - s_ag_{a}^{zz}(t)}{2} \right) \quad (9.58)
\]

\[
= \frac{1}{2} \sum_{\eta = \pm} \prod_{a \in \mathcal{S}} \left( \frac{1 + s_a \eta \sin^2 \theta_a + s_a \eta \cos^2 \theta_a \cos \omega_a t}{2} \right) \quad (9.59)
\]

\[
\sim \frac{1}{2} \left[ e^{-N \cos^2 \theta_0 \sin^2 \left( \frac{\omega_a t}{2} \right)} + e^{N \sin^2 \theta_0 - N \cos^2 \left( \frac{\omega_a t}{2} \right)} \right]. \quad (9.60)
\]

Note that in the above we only assumed \(\omega_a = \omega_0\), \(\theta_a = \theta_0\) and \(s_a = +1\) in the last step. Plots of \(p_c(t) = \text{tr} \hat{C}(t) \hat{C}_0\) are shown in figure 9.1. We see that when \(\theta_0\) is significantly less that \(\pi/2\) so that there is a significant transverse field on the spins there are peaks of \(p_c\) at multiples of the half the period of each qubit’s rotation as the transverse components of all the spins are tipped in and out of the \(z = 0\) plane. In between these peaks the return probability is vanishingly small for large \(N\). When \(\theta_0\) is close to zero there is a second set of peaks whose height is determined by \(\cos 2\phi\) this arises as when the field is entirely transverse. The second set of peaks comes from the qubits’ transverse polarisation components anti aligning after rotation of an angle of \(\pi\).

Correlators of the form \(\langle \prod_{a \in \mathcal{S} \setminus \mathcal{C}} \tau_a^x \prod_{b \in \mathcal{C}} \tau_b^y \rangle\) are interesting for diagnosing the off diagonal elements of the density matrix. These correlators have the following time dependence

\[
\langle \prod_{a \in \mathcal{S} \setminus \mathcal{C}} \tau_a^x \prod_{b \in \mathcal{C}} \tau_b^y \rangle(t) = \text{Re} e^{i\phi} \prod_{a \in \mathcal{S} \setminus \mathcal{C}} \frac{1}{g_{a}^{xx} - ig_{a}^{yy}} \prod_{b \in \mathcal{C}} \frac{1}{g_{b}^{xy} - ig_{b}^{yx}} + \prod_{a \in \mathcal{S} \setminus \mathcal{C}} g_{a}^{xx} \prod_{b \in \mathcal{C}} g_{b}^{yz} \quad (9.61)
\]

\[
= \text{Re} e^{i\phi} \prod_{a \in \mathcal{S} \setminus \mathcal{C}} \left[ \cos^2 \theta_a + \cos \omega_a t (1 - \cos^2 \theta_a) - i \sin \theta_a \sin \omega_a t \right] \nonumber
\]

\[
\times \prod_{b \in \mathcal{C}} \left[ - \sin \theta_b \sin \omega_b t - i \cos \omega_b t \right] + \prod_{a \in \mathcal{S} \setminus \mathcal{C}} \cos \theta_a \sin \theta_a \left[ 1 - \cos \omega_a t \right] \prod_{b \in \mathcal{C}} \cos \theta_b \sin \omega_b t. \quad (9.62)
\]

Now if \(N \gg 1\) it follows that at least one of \(\mathcal{C}\) and \(\mathcal{S} \setminus \mathcal{C}\) are large. For \(|\mathcal{C}| \gg 1\) and
Figure 9.1: Some plots of $p_c(t)$ for cat states in systems where all qubits have the same field. The solid (blue) line shows the exact expression (9.42) and the dotted (red) line shows the approximation (9.51), in (a) $N = 10$, $\theta_0 = 0$, in (b) $N = 10$, $\theta_0 = \frac{\pi}{4}$, in (c) $N = 10$, $\theta_0 = \frac{3\pi}{2}$, in (d) $N = 20$, $\theta_0 = 0$, in (e) $N = 20$, $\theta_0 = \frac{\pi}{4}$, and in (f) $N = 20$, $\theta_0 = \frac{3\pi}{2}$. In all cases we have set $\phi = \frac{\pi}{8}$. Note that the approximate formula works best close to the peaks but fails in between in particular the phase of the oscillating function is not well described by the approximate formula in between the peaks. Not shown is the case where $\theta_0 = \frac{\pi}{2}$ where we get a pure sinusoidal waveform.
\[ |S\setminus C| \gg 1 \text{ we have} \]
\[ \prod_{a \in S\setminus C} \left[ \cos^2 \theta_0 + \cos \omega_0 t (1 - \cos^2 \theta_0) - i \sin \theta_0 \sin \omega_0 t \right] \]
\[ \sim \sum_{\ell=0}^{\infty} e^{i(N-|C|)\xi_0 (t - \frac{2\pi \ell}{\omega_0}) - \frac{1}{32} (N-|C|) \sin^2 \theta_0 (\omega_0 t - 2\pi \ell)^4} \]
\[ \prod_{b \in C} [-\sin \theta_0 \sin \omega_0 t - i \cos \omega_0 t] \sim \sum_{\ell=0}^{\infty} e^{-\frac{|C|}{2} \cos^2 \theta_0 (\omega_0 t - \pi \ell)^2 + i|C|[t - \frac{\pi \ell}{\omega_0}] - \frac{\pi}{2} |C|} \]
\[ \prod_{a \in S\setminus C} \cos \theta_0 \sin \theta_0 [1 - \cos \omega_0 t] \sim e^{-\frac{N-|C|}{2} \cos^2 \theta_0 - (N-|C|) \cos^2 (\omega_0 t/2)} \]
\[ \prod_{b \in C} \cos \theta_0 \sin \omega_0 t \sim \text{sgn}(\sin |C| \omega_0 t) e^{-\frac{|C|}{2} \sin^2 \theta_0 - \frac{|C|}{2} \cos^2 \omega_0 t}. \]

Thus if both \(|C| \gg 1\) and \(|S\setminus C| \gg 1\) we have,
\[ \left\langle \prod_{a \in S\setminus C} \tau_a^x \prod_{b \in C} \tau_b^y \right\rangle (t) \]
\[ \sim \sum_{\ell=0}^{\infty} \cos \left[ N \sin \theta_0 (\omega_0 t - 2\pi \ell) + \phi - \frac{\pi}{2} |C| \right] \]
\[ \cdot e^{-\frac{1}{32} (N-|C|) \sin^2 \theta_0 (\omega_0 t - 2\pi \ell)^4 - \frac{|C|}{4} \cos^2 \theta_0 (\omega_0 t - 2\pi \ell)^2} \]
\[ + \text{sgn}(\sin |C| \omega_0 t) \]
\[ \cdot \exp \left\{ -\frac{|C|}{2} \sin^2 \theta_0 - \frac{|C|}{2} \cos^2 \omega_0 t - \frac{N-|C|}{2} \cos^2 \theta_0 - (N-|C|) \cos^2 (\omega_0 t/2) \right\}. \]

So each of the correlators oscillates in a similar way to the return probabilities. Plots of the off diagonal correlators in this case are shown in figure 9.2.

### 9.3.1 The Effect of Disorder

Now we can add the effect of the disorder in the Hamiltonian. We will start by considering the case where the field strength each qubit feels \(\{\omega_a\}\) are different. In general there are a large set of different parameter regimes that one can consider even in this simple case. We will specialise to the case where the histogram of field strengths \(\{\omega_a\}\) is sharply peaked around a mean value \(\omega_0\). This has the effect of spreading out each of the recurrences that occur in various quantities in the uniform case. For instance consider the expression for the off diagonal part of the return probability in the uniform case as long as the recurrences occur the same argument.
that lead to equation (9.51) leads to

\[
p_c(t) = \text{tr} \hat{C}(t) \hat{C}(0) \sim \frac{1}{2} \cos(2\phi)e^{-N\sin^2 \theta_0 - \frac{\omega a^2 t^2}{4}} 
+ \frac{1}{2} \cos \left( \sum \xi_a t + \vartheta(t) \right) e^{-\cos^2 \theta_0 \sum_a \sin^2 \left( \frac{\omega a^2 t}{2} \right)}
\] (9.69)

now unlike the uniform field case all of the \(\cos^2 \left( \frac{\omega a^2 t}{2} \right) = 0\) are not equal to zero at the same time. If we calculate this term at the \(n^{th}\) recurrence time \(t_n = \frac{(1+2n)\pi}{\omega_0}\) (putting \(\omega = \omega_0 + \delta \omega_a\) and expanding in \(t_n\delta \omega\)) we get \(\cos^2 \left( \frac{\omega a^2 t_n}{2} \right) \sim \frac{1}{4} \delta \omega_a^2 t_n^2\) thus the first term in (9.51) can be corrected by putting \(e^{-\sum_a \cos^2 \left( \frac{\omega a^2 t}{2} \right)} \rightarrow e^{-N\cos^2 \left( \frac{\omega_0 t}{2} \right) - \frac{N}{4} \delta \omega^2 t^2} \) with \(\delta \omega^2 \equiv \sum_a \delta \omega_a^2 / N\). Using this kind of approximation all terms in equation (9.51) one gets,

\[
p_c(t) = \text{tr} \hat{C}(t) \hat{C}(0) \sim \frac{1}{2} \cos(2\phi)e^{-N\sin^2 \theta_0 - N\cos^2 \left( \frac{\omega_0 t}{2} \right) - \frac{N}{4} \delta \omega^2 t^2} 
+ \frac{1}{2} \cos \left( \sum \xi_a t + \vartheta(t) \right) e^{-N\cos^2 \theta_0 \left[ \sin^2 \left( \frac{\omega_0 t}{2} \right) + \frac{\omega a^2 t}{4} \right] - \frac{N}{2} \sin^2 \theta_0 \delta \omega^2 t^2}.
\] (9.70)

Some plots of \(p_c(t)\) with disordered local field are shown in figure 9.3. As one would expect there is no decay when \(\theta_0 = \pi\) and the field is truly longitudinal we just see coherent oscillations at the frequency \(\sum_a \xi_a\).

The analogous expansion approximation for the off-diagonal correlators in the presence of disorder gives,

\[
\left< \prod_{a \in S \backslash C} \tau^x_a \prod_{b \in C} \tau^y_b \right>(t)
\sim \text{sgn} \left( \sin |C| \omega_0 t \right) e^{-\frac{|C|}{2} \sin^2 \theta_0 - \frac{|C|}{2} \cos^2 \omega_0 t - \frac{N-|C|}{2} \cos^2 2\theta_0 - (N-|C|) \cos^2 \left( \omega_0 t/2 \right)} 
+ e^{-\frac{1}{32} (N-|C|) \delta \omega^2 t^2} \left[ \cos^2 \theta_0 \omega_0 t - \sin^2 \theta_0 \omega_0 t \right] 
\cdot \sum_{t=0}^{\infty} \cos \left[ N \sin \theta_0 (\omega_0 t - 2\pi \ell) + \phi - \frac{\pi}{2} |C| \right] 
\cdot e^{-\frac{1}{32} (N-|C|) \sin^2 2\theta_0 (\omega_0 t - 2\pi \ell)^4 - \frac{|C|}{4} \cos^2 \theta_0 (\omega_0 t - 2\pi \ell)^2}
\] (9.71)

where we have defined the “moments” of \(\delta \omega_a\) over a set \(C\) by

\[
\overline{\delta \omega^2_C} = \sum_{a \in C} \delta \omega_a^2 / |C|\] (9.72)
\[
\overline{\delta \omega^4_C} = \sum_{a \in C} \delta \omega_a^4 / |C|.
\] (9.73)
We see from equation (9.71) that when \(|C| = \mathcal{O}(1)\) (and \(\theta_0 \approx \frac{\pi}{4}(2n+1)\) for \(n \in \mathbb{Z}\)) the component of \(\prod_{a \in S \setminus C} \tau_a \prod_{b \in C} \tau_b^y(t)\) which comes from the initial off-diagonal correlations dies down much slower with the disorder when compared to the component from the diagonal correlators. This does not contribute to the return probability as the phases of these different correlators mean their contributions to \(p_c(t)\) all cancel out. Plots of the off diagonal correlators in this case are shown in figure 9.2.

We have found that both the return probability and the amplitude of the different off-diagonal correlators all die down over time when we have disordered local fields even in the absence of an environment (this is of course on a time scale such that the recurrence times for the whole system are infinite). We know that the purity must be constant in an isolated system. What about the part of the purity contained in the off diagonal correlators? We find up to an exponentially small term

\[
p_{\perp S}(t) = \frac{1}{2} \prod_{a \in S} \left\{ \cos^2 \omega_a t + \sin^2 \theta_a \sin^2 \omega_a t + 2 \sin^2 \left( \frac{\omega_a t}{2} \right) \cos^2 \theta_a \left[ \sin^2 \left( \frac{\omega_a t}{2} \right) + 1 \right] \right\}
\]

\[
\sim \frac{1}{2} \left( e^{-\frac{N}{2} \cos^2 \theta_0 \delta \omega^2 t^2} - 2N \cos^2 \theta_0 \sin^2 (\omega_0 t/2) + e^{-8N \sin^2 (\theta_0/2) - (1+\cos \omega_0 t) - \frac{N}{2} \delta \omega^2 t^2} \right)
\]

(9.74)

(9.75)

which also decays over time unless the field is purely longitudinal. The total purity contained in the \(N\)th order correlators must be constant over time as there are no interaction terms in the Hamiltonian (9.37) so the decay of \(p_{\perp S}\) occurs when there is a transverse component to the local fields as the purity “contained” in the \(2^N\) \(N\)’th order correlators with components in the \(x - y\) plane is spread amongst all of the \(3^N\) \(N\)’th order correlators.

So far we have examined the effect of disorder in the local field strength felt by each qubit. Now we consider disorder in the orientation of the local field. First we will consider the case where all the fields have the same strength \(\omega_a = \omega_0\) and there is only a disorder in the angular variables. The effect of very weak disorder will be most dramatic when \(\theta_0 = \frac{\pi}{2}\) and the local fields are almost longitudinal, so that without disorder we would expect coherent oscillations at a frequency \(N \omega_0\) for the return probability. When we have disordered angles the generalisation of equation (9.51) for the large \(N\) off-diagonal return probability is,

\[
p_c(t) = \text{tr} \hat{C}(t) \hat{C}(0) \sim \frac{1}{2} \cos(2\phi) e^{-\sum_a \sin^2 \theta_a - N \cos^2 \left( \frac{\omega_0 t}{2} \right)}
\]

\[
+ \frac{1}{2} \cos \left( \sum \xi_a t + \vartheta(t) \right) e^{-\sum_a \cos^2 \theta_a \sin^2 \left( \frac{\omega_0 t}{2} \right)}.
\]

(9.76)

Thus we can write \(p_c(t)\) in terms of the averaged quantities \(\sum_a \sin^2 \theta_a = N \sin^2 \theta\),
Figure 9.2: Some plots of off diagonal correlators for cat states in system with \( N = 20 \) central qubits where all qubits feel a central field. The solid (blue) line shows the exact expression (9.42) and the dotted (red) line shows the approximation (9.71). Plot (a) shows \( \langle \Pi_a \tau^x_a \rangle \) without disorder, (b) shows \( \langle \Pi_a^N \tau^x_a \rangle \) where the central field strength has gaussian disorder characterised by the mean \( \delta \omega^2 = 0.05\omega_0 \), (c) shows \( \langle \Pi_a^N \tau^y_a \rangle \) without disorder and (d) shows \( \langle \Pi_a^N \tau^y_a \rangle \) where the central field strength has gaussian disorder characterised by the mean \( \delta \omega^2 = 0.05\omega_0 \). In all cases we have set \( \phi = 0 \) and all \( \theta_a = \theta_0 = \frac{\pi}{4} \).
Figure 9.3: Some plots of $p_c(t)$ for cat states in systems when there is a disordered central field strength. The solid line shows the exact expression (9.62) and the dashed line shows the approximations (9.70), in (a) $\sqrt{\delta \omega^2} = 0.01\omega_0, \theta_0 = 0$, in (b) $\sqrt{\delta \omega^2} = 0.01\omega_0, \theta_0 = \frac{\pi}{4}$, in (c) $\sqrt{\delta \omega^2} = 0.01\omega_0, \theta_0 = \frac{3}{8}\pi$, in (d) $\sqrt{\delta \omega^2} = 0.05\omega_0, \theta_0 = 0$, in (e) $\sqrt{\delta \omega^2} = 0.05\omega_0, \theta_0 = \frac{\pi}{4}$, and in (f) $\sqrt{\delta \omega^2} = 0.05\omega_0, \theta_0 = \frac{3}{8}\pi$. In all cases we have set $\phi = \frac{\pi}{4}$ and $N = 20$. The approximate formula works best from times such that $\delta \omega^2 t^2 \ll 1$, increasing $N$ makes the approximation better at longer times as it kills off the smaller oscillations. Not shown is the case where $\theta_0 = \frac{\pi}{2}$ where we get a pure sinusoidal waveform.
Figure 9.4: The configuration of the bath discussed in section 9.4, each central system qubit \( \{ \tau_a \text{ for } i = 1 \ldots N \} \) is coupled to its own set of bath spins \( B_a = \{ \sigma_{ai} \text{ for } i = 1 \ldots |B_a| \} \). We have illustrated the case where there are two central spins.

\[
\sum_a \cos^2 \theta_a = \frac{N \cos^2 \theta}{2} \quad \text{and} \quad \sum_a \xi_a = N \xi,
\]

\[
p_c(t) = \text{tr} \hat{C}(t) \hat{C}(0) \sim \frac{1}{2} \cos(2\phi)e^{-N \sin^2 \theta - N \cos^2(\frac{\omega_0 t}{2})}
+ \frac{1}{2} \cos(N \xi t + \varphi(t)) e^{-N \cos^2 \theta \sin^2(\frac{\omega_0 t}{2})}.
\]

The first term in the equation (9.77) is exponentially small so long as \( \sin^2 \theta \sim O(1) \) and peaks when \( \omega_0 t = \pi(2n + 1) \) for \( n \in \mathbb{Z} \). The second term in equation (9.77) is exponentially small for \( \cos^2 \theta \sim O(1) \) unless \( \omega_0 t = 2n\pi \) for \( n \in \mathbb{Z} \). So we see that disorder in the direction of the local fields changes the structure of the recurrences but in order to get decay of the amplitudes of these regular recurrences we need disorder in the strengths of the local fields so that we have a spread of the oscillation frequencies.

### 9.4 Degeneracy Blocking for a Large Cat State

Consider now a multi-qubit generalisation of the degeneracy blocking Hamiltonian from section 6.1,

\[
H = \sum_{a \in S} \frac{\Delta_a}{2} \tau_a^x + \sum_{a \in S} \sum_{i \in B_a} \frac{1}{2} \omega_{ai} \sigma_{ai}^x \tau_a^z.
\]

We will consider a case where the interactions between bath and central qubits is like that shown in figure 9.4. Each central spin \( \tau_a \) is coupled to its own bath of bath spins \( B_a \) so that the total bath is \( B = B_1 \cup B_2 \cup \ldots \cup B_N \). For simplicity we assume that the bath \( B_a \) belonging to each central spin \( \tau_a \) is the same size and the interactions between each central spin and its bath spins are the same, that is \( \omega_{ai} = \omega_i \). With an initial density matrix that is a product state \( \rho(0) = \rho_S(0)\rho_B(0) \) and the initial
reduced density matrix the central system $\rho_S(0)$ as the cat state \((3.41)\). We take
the initial reduced density for the bath separates $\rho_B(0) = \prod_a \rho_{B_a}(0)$ where each
$\rho_{B_a}(0) = \bar{\rho}_B(0)$ is the same.

As we saw in section \[6.1\] the only relevant part of $\rho_B$ for determining the dynamics of the central spin correlators is the part that contains information about the operator $\xi_a \equiv \sum_{i \in B_a} \omega_{ai} \sigma_z^a$, which commutes with the Hamiltonian. Thus if we are not interested in the time dependence of the bath correlators we can with out loss of generality consider a spectral decomposition of $\bar{\rho}_B(0)$ of the form,

$$\bar{\rho}_B(t) = \int_{-\infty}^{\infty} d\xi P^{\rho}_{DB}(\xi) \hat{\delta}(\xi - \xi_a).$$

Here $P^{\rho}_{DB}(\xi)$ acts as a time independent probability density for the bias field. Thus in this case the Green function for the single qubit correlations of qubit $a$ is

$$g_{\mu\nu}^a(t) = \int_{-\infty}^{\infty} d\xi P^{\rho}_{DB}(\xi) g_{\mu\nu}^a(t; \xi)$$

where

$$g_{\mu\nu}^a(t; \xi) = \cos^2 \theta_a(\xi) \hat{x}_\mu \hat{x}_\nu + \sin^2 \theta_a(\xi) \hat{z}_\mu \hat{z}_\nu + \cos \theta_a(\xi) \sin \theta_a(\xi) (\hat{x}_\mu \hat{z}_\nu + \hat{z}_\mu \hat{x}_\nu)
+ \cos \omega_\xi \xi \left[ (1 - \cos^2 \theta(\xi)) \hat{x}_\mu \hat{x}_\nu + (1 - \sin^2 \theta(\xi)) \hat{z}_\mu \hat{z}_\nu + \hat{y}_\mu \hat{y}_\nu
- 2 \cos \theta(\xi) \sin \theta(\xi) \theta (\hat{x}_\mu \hat{z}_\nu + \hat{z}_\mu \hat{x}_\nu) \right]$$

$$+ \sin \omega_\xi \xi \left( 2 \cos \theta(\xi) (\hat{y}_\mu \hat{z}_\nu - \hat{z}_\mu \hat{y}_\nu) + 2 \sin \theta(\xi) (\hat{x}_\mu \hat{y}_\nu - \hat{y}_\mu \hat{x}_\nu) \right)$$

$$\text{with: } \cos \theta(\xi) \equiv \frac{\xi}{\omega_\xi}$$

$$\omega_\xi \equiv \sqrt{\xi^2 + \Delta^2_a}.$$  \[9.83\]

The time evolution of the $N$ point correlator $C^{\mu_1...\mu_N}$ defined in the previous section is just

$$C^{\mu_1...\mu_N} = \prod_{a \in S} g^a_{\mu_\alpha \nu_\alpha} C^{N}_{\nu_1...\nu_N}$$

where $g^a_{\mu_\alpha \nu_\alpha}$ is the degeneracy averaged single spin Green function \[6.15\]. So that
the \( p_c(t) \) is

\[
\text{tr} \hat{C}(t) \hat{C}_0 = \frac{1}{2} \text{Re} \left\{ e^{2i\phi} \prod_a \frac{1}{2} \left[ g_a^{xx} - g_a^{yy} - i(g_a^{xy} + g_a^{yx}) \right] \right. \\
\left. + \prod_a \frac{1}{2} \left[ g_a^{xx} + g_a^{yy} - i(g_a^{xy} - g_a^{yx}) \right] \right\} \\
= \frac{1}{2} \text{Re} \left\{ e^{2i\phi} \prod_a \frac{1}{2} \int_{-\infty}^{\infty} d\xi_a P_{DB}^a(\xi_a) \left[ \cos^2 \theta_a (1 - \cos \omega_a t) \right] \\
+ \frac{1}{2} \prod_a \frac{1}{2} \int_{-\infty}^{\infty} d\xi_a P_{DB}^a(\xi_a) \left[ \cos^2 \theta_a + (2 - \cos^2 \theta_a) \cos \omega_a t - 2i \sin \theta_a \sin \omega_a t \right] \right\}. \\
\tag{9.85}
\]

Examine the two integrals appearing in the above expression with the assumption that the spectral density is an even function \( P_{DB}^a(\xi) = P_{DB}^a(-\xi) \) then we can write the above integrals as integrals over the frequency as follows,

\[
\frac{1}{2} \int_{-\infty}^{\infty} d\xi_a P_{DB}^a(\xi_a) \cos^2 \theta_a (1 - \cos \omega_a t) = \text{Re} \int_{\Delta_a} \frac{\Delta_a^2 P_{DB}^a(\sqrt{\omega^2 - \Delta_a^2})}{\omega \sqrt{\omega^2 - \Delta_a^2}} (1 - e^{i\omega t}) \\
\tag{9.86}
\]

\[
\frac{1}{2} \int_{-\infty}^{\infty} d\xi_a P_{DB}^a(\xi_a) \left[ \cos^2 \theta_a + (2 - \cos^2 \theta_a) \cos \omega_a t - 2i \sin \theta_a \sin \omega_a t \right] \\
= \int_{\Delta_a} \frac{P_{DB}^a(\sqrt{\omega^2 - \Delta_a^2})}{\omega \sqrt{\omega^2 - \Delta_a^2}} \left[ \Delta_a^2 + (2\omega^2 - \Delta_a^2) \cos \omega t - 2i\omega \sqrt{\omega^2 - \Delta_a^2} \sin \omega t \right]. \\
\tag{9.87}
\]

Which can be written as constant terms added to various Fourier integrals with an amplitude that is smooth except at \( \omega = \Delta_a \). Theorems in Fourier analysis [66] imply that the long time behaviour can be obtained by expanding the Fourier amplitudes around any points where they fail to be smooth so that the long time \( t \to \infty \) behaviour of the integrals appearing in (9.86) is

\[
\frac{1}{2} \int_{-\infty}^{\infty} d\xi_a P_{DB}^a(\xi_a) \cos^2 \theta_a (1 - \cos \omega_a t) \sim \frac{1}{2} \int_{-\infty}^{\infty} d\xi_a \frac{P_a(\xi_a) \Delta_a^2}{\xi_a^2 + \Delta_a^2} \\
- P_{DB}^a(0) \sqrt{\frac{\pi \Delta_a}{2t}} \cos \left( \Delta_a t + \frac{T}{4} \right) \\
\tag{9.89}
\]

\[
\frac{1}{2} \int_{-\infty}^{\infty} d\xi_a P_{DB}^a(\xi_a) \left[ \cos^2 \theta_a + (2 - \cos^2 \theta_a) \cos \omega_a t - 2i \sin \theta_a \sin \omega_a t \right] \\
\sim \frac{1}{2} \int_{-\infty}^{\infty} d\xi_a \frac{P_{DB}^a(\xi_a) \Delta_a^2}{\xi_a^2 + \Delta_a^2} + P_{DB}^a(0) \sqrt{\frac{\pi \Delta_a}{2t}} \cos \left( \Delta_a t + \frac{T}{4} \right). \\
\tag{9.90}
\]
Assuming all $\Delta_a = \Delta_0$, $P_{DB}^a(\xi_a) = P_{DB}(\xi_a)$ are the same, and defining $g_{xx}^{\infty} \equiv \frac{1}{2} \int_0^\infty d\xi_a P_{DB}(\xi_a) \Delta_0^2 \xi_a$. Then we get an approximate formula for the off-diagonal return probability in the long time limit.

$$p_c(t) \sim \cos 2\phi \left[ g_{\infty}^{xx} - P_{DB}(0) \sqrt{\frac{\pi \Delta_0}{2t}} \cos \left( \Delta_0 t + \frac{\pi}{4} \right) \right]^N$$

$$+ \left[ g_{\infty}^{xx} + P_{DB}(0) \sqrt{\frac{\pi \Delta_0}{2t}} \cos \left( \Delta_0 t + \frac{\pi}{4} \right) \right]^N$$

Now consider the case where we have a Gaussian density of bias fields with standard deviation $\delta \xi$,

$$P_{DB}(\xi_a) = e^{-\frac{\xi_a^2}{2\delta \xi^2}} \sqrt{\frac{2}{\pi \delta \xi}}. \quad (9.93)$$

in which case equation (9.91) becomes

$$p_c(t) \sim \cos 2\phi \left[ g_{\infty}^{xx} - \frac{1}{2} \sqrt{\frac{\Delta_0}{\delta \xi^2 t}} \cos \left( \Delta_0 t + \frac{\pi}{4} \right) \right]^N + \left[ g_{\infty}^{xx} + \frac{1}{2} \sqrt{\frac{\Delta_0}{\delta \xi^2 t}} \cos \left( \Delta_0 t + \frac{\pi}{4} \right) \right]^N$$

with

$$g_{\infty}^{xx} = \sqrt{\frac{\pi}{2}} \frac{\Delta_0^2}{2\delta \xi} e^{\frac{\Delta_0^2}{2\delta \xi}} \text{erfc} \left( \frac{\Delta_0}{\sqrt{2}\delta \xi} \right). \quad (9.95)$$

The approximation contained in equation (9.94) is tested in figure 9.5 where we see that when the standard deviation of the bath bias is small the approximation takes a long time to become accurate and even with a modestly large number of spins the return probability can be very small by the time the approximation is accurate. This is because in the expansion (9.94) one is assuming that all dimensionless parameters proportional to $t$ are large in particular one is assuming $\delta \xi t$ is large. This also explains why one does not obtain the $\delta \xi = 0$ result from sending $\delta \xi \to 0$ in equation (9.94). To remedy this one can calculate an approximation to the integrals (9.87-9.88) using the steepest descent method [7] in a way that takes into account the fact that $\delta \xi$ can be small. This approximation is derived in appendix F.1 instead of treating $t$ as a large parameter it treats $\sqrt{t^2 \delta \xi^2 + \frac{\Delta_0^2}{\delta \xi^2}}$ as a large parameter and
gives the following results for the integrals (9.87) (9.88)

\[
\frac{1}{2} \int_{-\infty}^{\infty} d\xi_a \frac{e^{-\frac{\xi^2}{2\delta^2}}}{\sqrt{2\pi\delta^2}} \cos^2 \theta_a (1 - \cos \omega_a t) \sim g^{xx}_{\infty} - \frac{1}{2} \cos \left( \frac{\Delta_a t + \frac{1}{2} \vartheta_a(t)}{\sqrt{1 + \frac{t^2\delta^4}{\Delta^4}}} \right)
\]

(9.96)

\[
\frac{1}{2} \int_{-\infty}^{\infty} d\xi_a \frac{e^{-\frac{\xi^2}{2\delta^2}}}{\sqrt{2\pi\delta^2}} \left[ \cos^2 \theta_a + (2 - \cos^2 \theta_a) \cos \omega_a t - 2i \sin \theta_a \sin \omega_a t \right]
\sim g^{xx}_{\infty} + \frac{1}{2} \cos \left( \frac{\Delta_a t + \frac{1}{2} \vartheta_a(t)}{\sqrt{1 + \frac{t^2\delta^4}{\Delta^4}}} \right)
\]

(9.97)

with: \( \tan \vartheta_a(t) = \frac{\delta \xi^2 t}{\Delta_0} \) (9.98)

\[ g^{xx}_{\infty} \sim \frac{1}{2} \sum_{n=0}^{\infty} (-2)^n \frac{\Gamma \left( \frac{1}{2} + n \right)}{\Gamma \left( \frac{1}{2} \right)} \left( \frac{\delta \xi}{\Delta_0} \right)^{2n} \] (9.99)

Therefore in this limit we have,

\[
p_c(t) \sim \cos 2\phi \left[ g^{xx}_{\infty} - \frac{1}{2} \cos \left( \frac{\Delta_a t + \frac{1}{2} \vartheta_a(t)}{\sqrt{1 + \frac{t^2\delta^4}{\Delta^4}}} \right) \right]^N + \left[ g^{xx}_{\infty} + \frac{1}{2} \cos \left( \frac{\Delta_a t + \frac{1}{2} \vartheta_a(t)}{\sqrt{1 + \frac{t^2\delta^4}{\Delta^4}}} \right) \right]^N.
\]

(9.100)

Figures [9.5] and [9.6] show the how the approximation works (9.100) we see it works well for longer times and that the errors present at shorter times are increased when \( N \) is increased. If \( N \) is large enough we see a regime where there are still coherent recurrences but the approximation (9.100) does not work as well as by the time the approximation is accurate \( p_c(t) \) is already negligible so we will have to work a bit harder to describe this region.

When \( N \) is very large we have seen that the approximation (9.100) will falls apart because the large exponents mean that the large product in equation (9.86) dies away much faster than each of the terms. We can get the amplitude of the “early” recurrences by noting that after a small number of periods the phase shift is negligible thus we can get the amplitude of the early peaks by evaluating the integrals in (9.86) at the times \( t_n = \frac{2\pi n}{\Delta_0} \) for integer \( n \) then expand in small \( \delta \xi \) yielding the following result for then height, \( p_{cn} \) of the \( n \)'th peak in the plot of \( p_c(t) \) (this requires \( \frac{\delta \xi}{\Delta} \ll 1 \) so that there are well defined peaks)

\[
p_{cn} \sim \frac{1}{2} e^{-\frac{3Nn^2\delta^4}{16\Delta_0}} \quad \text{for:} \quad \frac{t^2\delta^2}{\Delta_0} \ll 1.
\]

(9.101)
Figure 9.5: Some plots of $p_c(t)$ for cat states in systems with a simple degeneracy blocking spin bath. The solid line shows the exact expression (9.86), the dotted red line shows the long time approximation (9.94), and the dashed black line shows the long time small $\delta \xi$ approximation (9.100). In (a) $\delta \xi = 0.2\Delta_0$ and $N = 1$, in (b) $\delta \xi = 0.2\Delta_0$, $N = 5$, and the inset is the same plot magnified at earlier times, in (c) $\delta \xi = 0.1\Delta_0$ and $N = 1$, in (d) $\delta \xi = 0.1\Delta_0$, $N = 5$, and the inset is the same plot magnified at earlier times. In all cases we have set $\phi = \frac{\pi}{4}$. Note the difference in scale on the time axes between (a-b) and (c-d). We see in general the approximation (9.100) does a much better job when $\delta \xi$ is small for smaller times.
Which is plotted in figure 9.6 where we can see the cross over between the different regimes.

There is another limit which is worth considering, when either \( N \) or \( \delta \xi \) are large enough we only see the initial peak in the plot of \( p_c(t) \), in which case the \( p_c(t) \) can easily be calculated by expanding expressions in the small variable \( \Delta_0 t \) from which one finds

\[
p_c(t) \sim \frac{1}{2} e^{-\frac{N}{2} t^2 \left( \delta \xi^2 + \frac{1}{2} \Delta_0^2 \right)}.
\]  

(9.102)

So we see that the time dependence of \( p_c(t) \) can be divided into three regimes:

(i) In all cases there is a peak at \( t = 0 \) which will die away like \( \frac{1}{2} e^{-\frac{N}{2} t^2 \left( \delta \xi^2 + \frac{1}{2} \Delta_0^2 \right)} \) for times \( t \ll \Delta_0^{-1} \) and \( \delta \xi^{-1} \), (ii) the first few recurrences will occur at \( t = \frac{2 \pi n}{\omega_0} \) for \( n \in \mathbb{Z} \) and have an amplitude \( \sim \frac{1}{2} e^{-\frac{3}{4} \pi^2 N n \delta \xi^4} \) provided \( \frac{t \delta \xi^2}{\Delta_0^2} \ll 1 \) and will be visible if \( N \) is not to large compared to \( \frac{4 \delta \xi^2}{3 \omega_0^2 \Delta_0^2} \) and (iii) so long as \( \delta \xi \) is small enough there will also be a long time algebraic decay where \( p_c(t) \) is well approximated by (9.100). Note that in general for a given \( t > 0 \), \( p_c(t) \) scales with \( N \) like \( p_c \sim A(t) N \) for some \( A < 1 \) so that for any given time there is an \( N \) that will make \( p_c \) negligible at that time.

Now we look at the correlators in the limit where we can make the steepest descent approximation discussed in the appendix F.1. We have,

\[
\left\langle \prod_{a \in S \setminus C} \tau^x_a \prod_{b \in C} \tau^y_b \right\rangle(t) = \text{Re} \exp \int \prod_{b \in C} d\xi_b P(\xi_b) \left[ -\sin \theta_b \sin \omega_b t - i \cos \omega_b t \right].
\]

(9.103)

\[
\prod_{a \in S \setminus C} \int d\xi_a P(\xi_a) \left[ \cos^2 \theta_a + \cos \omega_a t (1 - \cos^2 \theta_a) - i \sin \theta_a \sin \omega_a t \right] \cdot \prod_{b \in C} \int d\xi_b P(\xi_b) \cos \theta_b \sin \omega_b t
\]

(9.104)

\[
\left\langle \prod_{a \in S \setminus C} \tau^x_a \prod_{b \in C} \tau^y_b \right\rangle(t) \sim \delta_{C,S} 2^N \left( 1 + \frac{t^2 \delta \xi^4}{\Delta^2} \right)^{-\frac{N}{4}} \sin^N \left( \Delta_0 t + \frac{1}{2} \vartheta \right) + \left( 1 + \frac{t^2 \delta \xi^4}{\Delta^2} \right)^{-\frac{|C|}{4}} \cos \left( \phi - \frac{\pi}{2} |C| \right) 2^{|C|} \cos^{|C|} \left( \Delta_0 t + \frac{1}{2} \vartheta \right) \cdot \left[ g_{\infty}^x + \frac{\delta \xi^2}{\sqrt{\Delta_0}} \left( t^2 \delta \xi^4 + \Delta_0^2 \right)^{-\frac{3}{4}} \cos \left( \Delta_0 t + \frac{3}{4} \vartheta \right) \right]^{N-|C|}.
\]  

(9.105, 9.106)
Figure 9.6: Some plots of $p_c(t)$ for cat states in systems with a simple degeneracy blocking spin bath. The solid line shows the exact expression (9.86) and the dotted red line shows the long time small $δξ$ approximation (9.100) and the dashed black line shows the approximation to the recurrence peak height (9.101). In (a) $δξ = 0.1\Delta_0$ and $N = 25$, in (b) $δξ = 0.1\Delta_0, N = 50$, in (c) $δξ = 0.1\Delta_0$ and $N = 100$, in (d) $δξ = 0.05\Delta_0, N = 25$, in (e) $δξ = 0.05\Delta_0, N = 50$, and in (f) $δξ = 0.05\Delta_0, N = 100$. In all cases we have set $ϕ = \frac{π}{4}$. We see in general the approximation (9.100) does a much better job when $δξ$ is small for smaller times.
The $\delta C_S$ term here is the contribution from the initial correlator $\langle \prod_{S} \tau_{z}^{i} \rangle$ and is only present when $N$ is even in which case the $z$ correlations can evolve into $y$ correlations only (this is a consequence of having a bias density which is symmetric around zero). So for long enough times correlators containing more $x$ components die off slower than those containing more $y$. In the case of the correlators the long time small $\delta \xi$ approximation works a lot better for large $N$. Plots of the off diagonal correlators in the degeneracy blocking case are shown in figure 9.7.

The off-diagonal purity in this degeneracy blocking case simplifies (the simple form is again due to the symmetry of the bias distribution $P_{DB}(\xi)$),

$$p_{S}(t) = \cos 2\phi \prod_{a} \left[ \frac{(g_{xx}^{a}(t))^{2} - (g_{yy}^{a}(t))^{2}}{1 + (g_{xx}^{a}(t))^{2} (g_{yy}^{a}(t))^{2}} \right]$$

$$\approx \frac{1}{2} \left\{ \cos 2\phi (g_{xx}^{a})^{N} \right\}$$

$$\frac{2}{(1 + (g_{xx}^{a}(t))^{2} (g_{yy}^{a}(t))^{2})^{1/4}}$$

$$+ \left[ \frac{(g_{xx}^{a})^{2} + \frac{1}{2} \cos (\Delta_{a}t + \frac{1}{2} \theta_{a}(t))}{1 + (g_{xx}^{a})^{2} (g_{yy}^{a})^{2}} \right]^{N}$$

One can also calculate the $N$-partite purity. I have omitted the expressions but produced plots in figure 9.8, where we see that the purity has decaying recurrences on top of a decaying “baseline” both of which decay in a similar way to the off-diagonal $p_{c}(t)$ (exponentially for small times or large enough $N$ and algebraically for long times).

### 9.5 General averaging

Now consider the case where each spin is coupled to its own bath so we still have a situation like that in figure 9.4 but with a more general bath Hamiltonian. As tracing out the bath acts like a form of averaging it is natural to consider the case where the effect of the bath is to average the Green function in a way which is analogous to (9.80). Indeed many central spin models (for example the precessional decoherence model discussed in chapter 7) reduce to finding a Green function for central spin $a$ of the form,

$$g_{a}^{\mu \nu}(t) = \int d^{n} \alpha g_{a}^{\mu \nu}(t; \alpha) P(\alpha)$$
Figure 9.7: Some plots of off diagonal correlators for cat states in system. The solid (blue) line shows the exact expression and the dotted (red) line shows the approximation (9.106). Plot (a) shows $\langle \prod_{a=1}^{N} \tau_{a}^{x} \rangle$ with $N = 25$ central qubits at $\delta \xi = 0.1 \Delta_0$, (b) shows $\langle \prod_{a=1}^{N} \tau_{a}^{y} \rangle$ with $N = 25$ central qubits at $\delta \xi = 0.1 \Delta_0$, (c) shows $\langle \prod_{a=1}^{N} \tau_{a}^{x} \rangle$ with $N = 101$ central qubits at $\delta \xi = 0.1 \Delta_0$, and (d) shows $\langle \prod_{a=1}^{N} \tau_{a}^{y} \rangle$ with $N = 101$ central qubits at $\delta \xi = 0.1 \Delta_0$. In all cases we have set $\phi = \frac{\pi}{4}$. 
Figure 9.8: Some plots of $p_S(t)$ for cat states in systems with a simple degeneracy blocking spin bath. In (a) $\delta \xi = 0.2\Delta_0$ and $N = 5$, in (b) $\delta \xi = 0.2\Delta_0, N = 25$, and the inset is the same plot magnified at earlier times, in (c) $\delta \xi = 0.1\Delta_0$ and $N = 25$, in (d) $\delta \xi = 0.1\Delta_0, N = 100$. 
where \( g^\mu\nu_a(t; \alpha) \) is the Green function for central spin \( a \) defined in terms of an \( n \) dimensional set of parameters \( \alpha = (\alpha_1, \alpha_2 \ldots \alpha_n) \) which are then averaged over with some weight function \( P(\alpha) \). In some cases (including all those listed above) \( g^\mu\nu_a(t; \alpha) \) will be expressible in terms of the Green function for a central spin in a simple field \( H_a = \frac{1}{2} \Omega(\alpha) \hat{n}(\alpha) \) (we can always chose \( \hat{n}(\alpha) \) so that \( \Omega(\alpha) > 0 \) so that

\[
g^\mu\nu_a(t; \alpha) = \hat{n}^\mu(\alpha) \hat{n}^\nu(\alpha) + [\hat{\delta}^\mu\nu - \hat{n}^\mu(\alpha) \hat{n}^\nu(\alpha)] \cos[\Omega(\alpha)t] + \sin[\Omega(\alpha)t] \varepsilon^{\mu\nu\lambda} \hat{n}_\lambda(\alpha).
\]

(9.110)

Then the average \( \langle 9.109 \rangle \) takes can be split into two different parts: (i) an even function of time

\[
g^\mu\nu_{a1}(t) = \int d^n \alpha P(\alpha) \hat{n}^\mu(\alpha) \hat{n}^\nu(\alpha) + \int d^n \alpha P(\alpha) [\hat{\delta}^\mu\nu - \hat{n}^\mu(\alpha) \hat{n}^\nu(\alpha)] \cos[\Omega(\alpha)t]
\]

(9.111)

\[
= g^\mu\nu_{a0} + \int d\omega \cos(\omega t) g^\mu\nu_{a2}(\omega)
\]

(9.112)

\[
g^\mu\nu_{a1}(\omega) = \int d^n \alpha P(\alpha) [\hat{\delta}^\mu\nu - \hat{n}^\mu(\alpha) \hat{n}^\nu(\alpha)] \delta(\Omega(\alpha) - \omega)
\]

(9.113)

\[
g^\mu\nu_{a0} = \int d^n \alpha P(\alpha) \hat{n}^\mu(\alpha) \hat{n}^\nu(\alpha)
\]

(9.114)

this also has eigenvalues which are less than one and (ii) an odd function of time \( \varepsilon^{\mu\nu\lambda} g^\lambda_{a2}(t) \),

\[
g^\mu_{a2}(t) = \int d^n \alpha P(\alpha) \sin[\Omega(\alpha)t] \hat{n}^\mu(\alpha) = \int_0^\infty d\omega g^\mu_{a2}(\omega) \sin(\omega t)
\]

(9.115)

\[
g^\mu_{a2}(\omega) = \int d^n \alpha P(\alpha) \hat{n}^\mu(\alpha) \delta(\Omega(\alpha) - \omega)
\]

(9.116)

which is the alternating tensor multiplied by a vector with length less than or equal to one. In the long time limit the behaviour of \( g^\mu\nu_a(t) \) will be dominated by any parts of the tensors \( g^\mu_{a1}(\omega) \) and \( g^\mu_{a2}(\omega) \) which fail to be analytic and the Green function will decay to a constant symmetric tensor \( g^\mu\nu_{a\infty} = \lim_{t \to \infty} g^\mu\nu_{a1}(t) \) which will have positive eigenvalues less than one. In the orthogonality blocking case above the \( g^\mu_{a2} = 0 \) and \( g^\mu_{a1}(\omega) \) has an isolated singularity at \( \omega = \Delta_0 \) at that singularity different components of \( g^\mu_{a2}(\omega) \) go like \( (\omega - \Delta_0)^{-\frac{1}{2}} \Theta(\omega - \Delta_0), \Theta(\omega - \Delta_0), \sqrt{\omega - \Delta_0} \Theta(\omega - \Delta_0) \) and \( (\omega - \Delta_0) \Theta(\omega - \Delta_0) \) which leads to the long time algebraic decay in the oscillations seen in the previous section. The probability density function in the orthogonality blocking example above \( P \to P_{DB}(\xi) = e^{-\xi^2/2\delta^2}/\sqrt{2\pi\delta^2} \) is well behaved enough that we can find an approximation that combines the long time behaviour using a steepest descent approximation. As we will see probability densities which do not have an exponential decay will require a different approach. In general for the above type of averaging without interactions between the central spins we will have for our
generalised cat states,

\[ \hat{C}(t) = \frac{1}{2^N} C_{\mu_1...\mu_n}^S(t) \prod_{a \in S} \tau_a^{\mu_a} \]  
(9.117)

\[ C_{\mu_1...\mu_n}^S(t) = \frac{1}{2} \text{Re} \, e^{i\phi} \prod_{a \in S} \left[ g_a^{\mu_a x}(t) - is_a g_a^{\mu_a y}(t) \right] \]  
(9.118)

\[ p_c(t) = \frac{1}{2} \text{Re} e^{2i\phi} \prod_{a \in S} \left[ g_a^{\mu_a x}(t) - is_a g_a^{\mu_a y}(t) \right] + \frac{1}{2} \text{Re} \prod_{a \in S} \left[ g_a^{\mu_a x} + g_a^{\mu_a y} - is_a g_a^{\mu_a z} \right] \]  
(9.119)

\[ p_c = \frac{1}{2} \text{Re} e^{2i\phi} \prod_{a \in S} \left[ g_a^{\mu_a x} - g_a^{\mu_a y} - 2is_a g_a^{\mu_a x} g_a^{\mu_a y} \right] + \frac{1}{2} \prod_{a \in S} \left[ g_a^{\mu_a x} g_a^{\mu_a y} - g_a^{\mu_a y} g_a^{\mu_a y} \right] \]  
(9.120)

\[ p_{\perp c} = \frac{1}{2} \text{Re} e^{2i\phi} \prod_{a \in S} \left[ \left( g_a^{\mu_a x} \right)^2 - \left( g_a^{\mu_a y} \right)^2 + 4g_a^{\mu_a x} g_a^{\mu_a y} - 2is_a \left( g_a^{\mu_a x} g_a^{\mu_a y} + g_a^{\mu_a y} g_a^{\mu_a x} \right) \right] \]  
\[ + \frac{1}{2} \prod_{a \in S} \left[ \left( g_a^{\mu_a x} \right)^2 + \left( g_a^{\mu_a y} \right)^2 + \left( g_a^{\mu_a y} \right)^2 \right] . \]  
(9.121)

Where we have assumed \( N \) is even. When \( N \) is odd the last term in equation (9.120) should be omitted.

### 9.5.1 Spherically Symmetric Degeneracy Blocking

Consider the slightly generalised version of the degeneracy blocking spin bath where the \( z \) components of the bath spins are allowed to couple to any component of the central spin,

\[ H = \sum_{a \in S} \frac{\Delta_a}{2} \tau_a^x + \sum_{a \in S, i \in B_a} \omega_{ai} \sigma_a^x \mathbf{m}_i \cdot \tau_a. \]  
(9.123)

in the same limit discussed above the field on each central spin is of the form \( \Delta_a \hat{x} + \xi_a = \Omega(\xi_a) \hat{n}(\xi_a) \) where \( \xi_a \) is a three dimensional vector drawn from some distribution \( P(\xi_a) \). \( \Omega(\xi_a) \) and \( \hat{n}(\xi_a) \) are in this case,

\[ \Omega(\xi_a) = \sqrt{(\Delta_a + \xi_x)^2 + \xi_y^2 + \xi_z^2} \]  
(9.124)

\[ \hat{n}(\xi_a) = \frac{\Delta_a \hat{x} + \xi_a}{\Omega(\xi_a)} \]  
(9.125)

A simple assumption is that \( P(\xi_a) \) is a spherically symmetric Gaussian distribution,

\[ P(\xi_a) = \frac{e^{-\xi_a^2/2\delta^2}}{(2\pi \delta^2)^3/2}. \]  
(9.126)
In this case the tensors $g_{a1}^\mu(\omega)$ and $g_{a2}^{\mu\nu}(\omega)$ are easily resolved in the “spherical polar co-ordinates” $\xi_x = \Omega \cos \theta - \Delta_\alpha$, $\xi_y = \Omega \sin \theta \cos \phi$, $\xi_z = \Omega \xi_y = \Omega \sin \theta \cos \phi$,

$$g_{a1}(\omega) = \omega^2 \frac{2\pi e^{-(\omega^2+\Delta^2)/2\delta^2}}{(2\pi \delta \xi^2)^{3/2}} \int_0^\pi d\theta \sin \theta e^{\omega \Delta \cos \theta / \delta^2} \begin{pmatrix} 1 - \cos^2 \theta & 0 & 0 \\ 0 & 1 - \frac{1}{2} \sin^2 \theta & 0 \\ 0 & 0 & 1 - \frac{1}{2} \sin^2 \theta \end{pmatrix} \frac{d\tilde{\omega}}{\omega^2}$$

$$= \omega^2 \frac{2\pi e^{-(\omega^2+\Delta^2)/2\delta^2}}{(2\pi \delta \xi^2)^{3/2}} \int_{-1}^1 du \frac{d\tilde{\omega}}{\delta \xi^2} \begin{pmatrix} 1 - u^2 & 0 & 0 \\ 0 & \frac{1}{2}(1 + u^2) & 0 \\ 0 & 0 & 1 - \frac{1}{2}(1 + u^2) \end{pmatrix} \frac{d\tilde{\omega}}{\omega^2}$$

$$g_{a2}(\omega) = \hat{x} \omega^2 \frac{2\pi e^{-(\omega^2+\Delta^2)/2\delta^2}}{(2\pi \delta \xi^2)^{3/2}} \int_0^\pi d\theta \sin \theta e^{\omega \Delta \cos \theta / \delta^2} \frac{d\tilde{\omega}}{\omega^2}$$

$$= \hat{x} \omega^2 \frac{2\pi e^{-(\omega^2+\Delta^2)/2\delta^2}}{(2\pi \delta \xi^2)^{3/2}} \int_{-1}^1 du \frac{d\tilde{\omega}}{\delta \xi^2} \begin{pmatrix} 1 - u^2 & 0 & 0 \\ 0 & \frac{1}{2}(1 + u^2) & 0 \\ 0 & 0 & 1 - \frac{1}{2}(1 + u^2) \end{pmatrix} \frac{d\tilde{\omega}}{\omega^2}$$

of which the only non-zero matrix elements are,

$$g_{a1}^{xx}(\omega) = \frac{\delta \xi}{\Delta_0^2} \sqrt{\frac{2}{\pi}} \left[ e^{-\frac{(\omega-\Delta_0)^2}{2\delta^2}} (\delta^2 + \Delta_0 \omega) + e^{-\frac{(\omega+\Delta_0)^2}{2\delta^2}} (\delta^2 - \Delta_0 \omega) \right]$$

$$g_{a1}^{yy}(\omega) = g_{a1}^{zz}(\omega)$$

$$= \frac{1}{\sqrt{2\pi} \Delta_0 \omega \delta \xi} \left[ e^{-\frac{(\omega+\Delta_0)^2}{2\delta^2}} (\delta^4 + \Delta_0^2 \omega^2 - \Delta_0 \omega \delta \xi^2) 
- e^{-\frac{(\omega-\Delta_0)^2}{2\delta^2}} (\delta^4 + \Delta_0^2 \omega^2 + \Delta_0 \omega \delta \xi^2) \right]$$

$$g_{a2}^{xx}(\omega) = \frac{1}{\sqrt{2\pi} \Delta_0^2} \left[ e^{-\frac{(\omega+\Delta_0)^2}{2\delta^2}} (1 - \Delta_0 \omega \delta \xi^2) - e^{-\frac{(\omega-\Delta_0)^2}{2\delta^2}} (1 + \Delta_0 \omega \delta \xi^2) \right].$$

these are smooth functions for all real frequencies so that their Fourier transforms are exponentially decaying oscillations with an underlying frequency of $\Delta_0$ (the peaks of the Fourier amplitudes),

$$g_{a1}^{xx}(t) = g_{a0}^{xx} + \frac{\Delta_0^2 e^{-\frac{\delta \xi^2 t}{2}}} {\Delta_0^2} \cos \Delta_0 t$$

$$g_{a1}^{yy}(t) = g_{a0}^{yy} + \frac{e^{-\frac{\delta \xi^2 t}{2}}}{\Delta_0^2} \left[ (\Delta_0^2 + \delta \xi^2) \cos \Delta_0 t + t \Delta_0 \delta \xi^2 \sin \Delta_0 t \right]$$

$$g_{a2}^{xx}(t) = e^{-\frac{\delta \xi^2 t}{2}} \left[ \Delta_0 \delta \xi^2 \cos \Delta_0 t + (\Delta_0^2 - \delta \xi^2) \sin \Delta_0 t \right].$$
9.5.2 Precessional Decoherence

Now we discuss the many qubit version of the precessional decoherence model discussed in section 7.2, we make the same assumptions about the initial conditions of the bath which we did in that section. In this case the dynamics of the bath on each spin are accounted for by performing an average of over an auxiliary variable $X$ with $\Omega(x) = \Delta_0 | J_0 (2X \sqrt{\kappa}) |$, $\hat{n}(x) = \hat{x}$ and $P(X) = X e^{-\frac{x^2}{4\kappa}}$ where $\kappa$ is the precessional decoherence variable defined in equation 7.67. The tensors, $g_{a_1}^{\mu \nu} (\omega)$ and $g_{a_2}^{\mu \nu} (\omega)$, in this case are

\begin{align*}
 g_{a_1}^{\mu \nu} (\omega) &= 2(\delta^{\mu \nu} - \hat{x}^\mu \hat{x}^\nu) \int_0^\infty \frac{dX}{4\kappa} X e^{-\frac{x^2}{4\kappa}} \delta(\Delta_0 J_0(X) - \omega) \\
 g_{a_2}^{\mu \nu} (\omega) &= 2\hat{x}^\mu \int_0^\infty \frac{dX}{4\kappa} X e^{-\frac{x^2}{4\kappa}} \delta(\Delta_0 J_0(X) - \omega).
\end{align*}

With the aid of the delta function identity $\delta(f(X)) = \delta(X)/|f'(X)|$, we can conclude that $g_{a_1}^{\mu \nu} (\omega)$ and $g_{a_2}^{\mu \nu} (\omega)$ fail to be smooth whenever $\omega = \Delta_0 J_0 (j_{0,m}')$, ($j_{0,m}'$ is the $m$th zero of the derivative of the $J_0(X)$ and $m = 0, 1, 2 \ldots$). $g_{a_1}^{zz} (\omega)$ is shown in figure 9.9 from which we can see that when $\kappa \ll 1$, the only non-analytic point that is significant is $\omega = \Delta_0 J_0 (0) = \Delta_0$. This is because the amplitude of the contribution to $g_{a_1}^{zz} (\omega)$ from at $j_{0,m}'$ is $\sim e^{-\frac{(j_{0,m}')^2}{4\kappa}}$ for small $\kappa$ and in that limit only the first zero $j_{00}'$ contributes.
So for small $\kappa$ we get

$$
\int_0^{\infty} \frac{dX}{4\kappa} X e^{-\frac{X^2}{4\kappa}} \delta(\Delta_0 J_0(X) - \omega)
= \int_0^{j_{01}} \frac{dX}{4\kappa} X e^{-\frac{X^2}{4\kappa}} \delta(\Delta_0 J_0(X) - \omega) + O \left(e^{-j_{01}/4\kappa}\right)
$$

$$
= \frac{J_{00}^{-1} \left( \frac{\omega}{\Delta_0} \right) \Theta(\Delta_0 - \omega) \Theta(\omega)}{\Delta_0 \kappa J_1 \left[ J_{00}^{-1} \left( \frac{\omega}{\Delta_0} \right) \right]} \exp \left\{ - \left[ \frac{J_{00}^{-1} \left( \frac{\omega}{\Delta_0} \right)^2}{4\kappa} \right] \right\} + O \left(e^{-j_{01}/4\kappa}\right). \quad (9.141)
$$

Here $J_{00}^{-1}(X)$ is the inverse function of the $J_0(X)$, defined by $J_{00}^{-1}(J_0(X)) = X$, on the domain $0 < X < j_{01}$, and $j_{01} \approx 2.4048$ is the first zero of $J_0(x)$. Then performing a steepest descent calculation like that in appendix F.1 gives us,

$$
g_{a1}^{\mu \nu}(t) \sim \hat{x}^\mu \hat{x}^\nu + (\delta^{\mu \nu} - \hat{x}^\mu \hat{x}^\nu) \frac{\cos \Delta_0 t + \Delta_0 t \kappa \sin \Delta_0 t}{\sqrt{1 + \kappa^2 \Delta_0^2 t^2}} \quad (9.142)
$$

$$
g_{a2}^{\mu}(t) \sim \hat{x}^\mu \frac{\sin \Delta_0 t - \Delta_0 t \kappa \cos \Delta_0 t}{\sqrt{1 + \kappa^2 \Delta_0^2 t^2}}. \quad (9.143)
$$

One then finds the correlators for cat state initial conditions,

$$
\left\langle \prod_{a \in C} \tau^a_x \prod_{b \in C} \tau^b_y \right\rangle = \cos \left( \phi - \frac{\pi}{2} |C| \right) \frac{\cos |C| \left( \Delta_0 t + \vartheta_{\kappa}(t) \right)}{(1 + \kappa^2 \Delta_0^2 t^2)^{|C|/2}} \quad (9.144)
$$

$$
tan \vartheta_{\kappa}(t) = \kappa \Delta_0 t. \quad (9.145)
$$

so we see in the lowest order orthogonality blocking approximation, $\tau^a_x$ is conserved (as discussed in section 7.2.3). The off diagonal return probability

$$
p_c(t) = \frac{1}{2N} \cos 2\phi \left( 1 - \frac{\cos \left( \Delta_0 t + \vartheta_{\kappa}(t) \right)}{\sqrt{1 + \kappa^2 \Delta_0^2 t^2}} \right)^N + \frac{1}{2N} \left( 1 + \frac{\cos \left( \Delta_0 t + \vartheta_{\kappa}(t) \right)}{\sqrt{1 + \kappa^2 \Delta_0^2 t^2}} \right)^N. \quad (9.146)
$$

We see that this is similar to the behaviour in the degeneracy blocking case, in the limit we have looked the key piece of information that determines the long time behaviour in the small $\kappa$ limit is the exponent close to $\omega = \Delta_0$ and the discontinuity of the Fourier tensors $g_{a1}^{\mu \nu}(\omega)$ and $g_{a2}^{\mu}(\omega)$ at this point.

### 9.5.3 Degeneracy Blocking with a Lorentzian Field Distribution

Consider the example in section 9.4 but with the bias weighting function,

$$
P_{\text{DB}}(\xi) = \frac{\gamma}{\pi(\gamma^2 + \xi^2)} \quad (9.147)
$$
which has ill defined moments. We can still obtain the long time behaviour by expanding the Fourier tensors $g_{n1}^{\mu\nu}(\omega)$ and $g_{n2}^{\mu\nu}(\omega)$ around their $\omega = \Delta_0$ values but this gives an expression which is only valid for large $\gamma t$ so if we want to include the possibility of $\gamma$ being small we will have to derive another expression. The steepest descents approach we used in section 9.4 does not work well here as we cannot treat the probability distribution as a term which varies exponentially fast with small $\gamma$ and modify the contour of integration appropriately. The problem is that as $\gamma \to 0$ the two poles in $P_{DB}(\xi)$ at $\xi = \pm i\gamma$ come closer and closer to the real axis. So any approximations which will be valid for small $\gamma t$ need to have the poles treated properly, in practice as the Green function has branch points at $\xi = \pm \Delta_0$ this means an approximation derived for small $\gamma$ will break down when $\gamma \sim \Delta_0$. Such an approximation is derived in the appendix F.2. The long time decay of various quantities is algebraic still but the short time behaviour is now non-analytic, a plot of $p_c(t)$ is shown in figure 9.10.

9.6 Conclusion

In this chapter we have presented some results for the dynamics of entangled states containing a large number of central qubits, which may be coupled to a bath. We have limited our discussion to cases where the central qubits do not interact either
directly or through a bath. We hope to tackle the interacting problem in future
work.

First in section 9.1 we discussed some simple ways to characterise these states,
based on their correlators, as they evolve from their initial values. Then in section
9.2 and 9.3 we studied their dynamics under the influence of only local fields. We
saw that if the fields were uniform then the motion could be characterised by dif-
ferent recurrences, and disorder could cause various recurrence amplitudes to decay,
even without interactions which change the amount of information stored in the
different orders of correlators. Then in sections 9.4 and 9.5 we considered some
examples where spin baths had to be averaged out. We found we could get results
by investigating the averaged single qubit Green function’s spectral properties and
that in general, when there are many central qubits, care needed to be taken to
obtain the correct asymptotic behaviour for high order correlators.
Chapter 10

Conclusions

Here we discuss the new work results presented in this thesis, and how we it could be extended.

In chapters 2 and 3 showed how we can understand multipartite entanglement as correlations. In this picture of entanglement, the different types of entanglement are be specified by different correlated parts of the reduced density matrices or by correlations between different clusters of qubits. We saw that the use of these decompositions is in many ways a more transparent way of characterising multipartite entanglement than the entanglement measures that have been discussed in the literature.

In particular in chapter we identified multiple different ways of splitting the many body density matrix into “correlated parts”, as an expansion over different entangled sets of the system, using $\hat{\rho}_A^C$ and, over different partitions of the system into entangled sets using $\hat{\rho}_{AC}^{CC}$. It would be interesting to see whether more precise connections between $\hat{\rho}_A^C$, $\hat{\rho}_{AC}^{CC}$ and the formal measures of entanglement can be made.

Then we focused on gaining an understanding the time evolution of multipartite entanglements, an important problem for the construction of a quantum computer. First we considered a formal approach to quite general problems involving pairwise interactions. In chapter 4 we showed correlated parts of the reduced density matrix $\hat{\rho}_A^C$, can be used to study the dynamics of the reduced density matrix, in cases when there are general pairwise interactions and we derived a hierarchy of equations of motion for many-body density matrices. We then saw that in the qubit case with only pairwise interactions and local fields included, there is a hierarchy of equations of motion for the qubit correlators, which links correlators containing a cluster of spins to correlators containing that cluster with one spin added or removed. When things are rewritten in terms of supervectors of qubit correlators, we found that the resulting matrix equations of motion involve sparse matrices, making them practically useful. It remains to be seen under what circumstances one could derive similar hierarchies of equations for the correlated parts of reduced density matrices or connected correlators between spin components, and whether they can be put in a useful form.

This work showed that the structure of the hierarchy of equations of motion implied that the information lost by a central qubit into a bath of spins is transferred to larger and larger correlators between the central qubit and bath spins, in a cascade
of coherence. We saw cascade exists this both in the simple degeneracy blocking model studied in chapter 6 and in the more realistic precessional decoherence model studied in chapter 7. This presents an intuitive way of understanding the important process of decoherence. It would be interesting to see how this cascade works in other situations, it is clear that while the details of this cascade might be different in other models, this picture is somewhat generic.

We showed how the cascade works out for the specific example of an Fe₈ magnetic molecule qubit in chapter 8. We investigated under what conditions one could expect to see signs of this cascade, if we could measure the correlators between pairs of bath spins and the central spin.

Finally in chapter 9 we studied the decay of entanglement in non-interacting models with many central spins, and saw the effect of large numbers in this case. We saw that the correlators responsible for N—partite entanglement decayed at a rate N times greater than a single central qubit. This places limitations on the construction of quantum computers which require the information in multipartite entanglement to function. An obvious avenue for future work is to extend this analysis to interacting systems with many qubits. It would be interesting to see how the information stored in many central qubit correlators is lost to the environment, when there are direct interactions between the central qubits or when the central qubits interact with a common bath. It is not clear how the cascade would work in these cases, information will not just be lost into correlators with containing bath spins, it will also be transferred to correlators containing different numbers of central spin. Understanding this cascade could lead to important insights into understanding the limitations of a many qubit quantum computer.
Bibliography


Appendix A

Properties of Entanglement Density Matrices

In this Appendix we prove two properties of the entanglement density matrices that were quoted without proof in section 2.0.3. We use same notation as that defined in this section.

A.1 Proof of Eqtn. (2.23)

We wish here to prove the result given in eqtn. (2.22) (or, equivalently eq. (2.23)) for the entanglement correlated density matrices.

We do this by induction. The $n = 2$ case comes from tracing out all of $S$ except $i$ and $j$ from the equation for the density matrix (2.2), so that

$$\bar{\rho}_{ij} = \bar{\rho}_{i} \bar{\rho}_{j} + \bar{\rho}_{ij}^C \Rightarrow \bar{\rho}_{ij}^C = \bar{\rho}_{ij} - \bar{\rho}_{i} \bar{\rho}_{j} \quad (A.1)$$

as required. Now we make the inductive assumption that for all $k < n$ and $B_k \subset A_n$ we have

$$\bar{\rho}_{B_k}^C = \sum_{m=2}^{k} (-1)^{(k-m)} \sum_{C_m \subseteq B_k} \left( \bar{\rho}_{C_m} \prod_{j \in B_k \setminus C_m} \bar{\rho}_{j} \right) - (-1)^k (k-1) \prod_{j \in B_k} \bar{\rho}_{j}. \quad (A.2)$$

Substituting equation (A.2) into

$$\bar{\rho}_{A_n} = \prod_{j \in A_n} \bar{\rho}_{j} + \bar{\rho}_{A_n}^C + \sum_{k=2}^{n-1} \sum_{C_k \subseteq A_n} \left( \prod_{j \in A_n \setminus C_k} \bar{\rho}_{j} \right) \bar{\rho}_{C_k}^C \quad (A.3)$$

then gives an expression of the form

$$\bar{\rho}_{A_n}^C = \bar{\rho}_{A_n} + \sum_{\ell=2}^{n-1} \sum_{\mathcal{F}_\ell \subseteq A_n} \xi_{\ell} \bar{\rho}_{\mathcal{F}_\ell} \prod_{i \in A_n \setminus \mathcal{F}_\ell} \bar{\rho}_{i} + \xi_0 \prod_{i \in A_n} \bar{\rho}_{i}. \quad (A.4)$$

This is because terms in (A.3) contain one $\bar{\rho}_{C_k}^C$ multiplied by the single cell reduced density matrices for the rest of the cells, and terms in (A.2) contain one
reduced density matrix over a larger set multiplied by single cell reduced density matrices, and all subsets of the same size appear symmetrically in (A.3) and (A.2). Thus the final expression is a sum over terms which are the product of a single reduced density matrix over a set \( F_\ell \subseteq A_n \) multiplied by single cell reduced density matrices with a coefficient depending only on the size \( \ell \) of the set \( F_\ell \). Now we need to find \( \xi_\ell \) and \( \xi_0 \).

To find \( \xi_\ell \) we note that every \( B_k \supseteq F_\ell \) \((B_k \subset A_n)\) gives a contribution \(-(-1)^{k-\ell}\) to \( \xi_\ell \), so there are \( n-\ell \binom{n}{k} \) such \( B_k \)'s for a given \( k \); thus the coefficient is

\[
\xi_\ell = - \sum_{k=\ell}^{n-1} (-1)^{k-\ell} \binom{n-\ell}{\ell} = - \sum_{p=0}^{n-\ell-1} (-1)^p \binom{n-\ell}{p}
\]

\[
= - \sum_{p=0}^{n-\ell} (-1)^p \binom{n-\ell}{p} + (-1)^{n-\ell} \binom{n-\ell}{n-\ell} = - (1 - 1)^{n-\ell} + (-1)^{n-\ell} = (-1)^{n-\ell}
\]

(A.5)

as required.

To find \( \xi_0 \) we note that there is a contribution \(-1\) from the first term in equation (A.3) as well as a contribution \((-1)^k(k - 1)\) from every \( B_k \) with \( n - 1 \geq k \geq 2 \). There are \( n \binom{n}{k} \) different \( B_k \)'s for each \( k \), so that

\[
\xi_0 = - 1 + \sum_{k=2}^{n-1} (-1)^k (k - 1) \binom{n}{k}
\]

\[
= (-1)^{n+1} (n - 1)
\]

(A.6)

as required; this completes the proof.

**A.2 Proof that any partial trace of \( \bar{\rho}_{A_n}^C \) is zero**

In the main text we took the result in eqtn. (2.9) to be a defining property of the partial trace. However, one can also derive the result explicitly from the expression (2.23). We now show this.

Let us begin with (2.23) of the main text, viz.,

\[
\text{tr}_i \bar{\rho}_{A_n}^C = \sum_{m=2}^{n} (-1)^{n-m} \sum_{\mathcal{C}_m \subseteq A_n} \text{tr}_i \left( \bar{\rho}_{\mathcal{C}_m} \prod_{j \in A_n \setminus \mathcal{C}_m} \bar{\rho}_j \right) - (-1)^n (n - 1) \prod_{j \in A_n \setminus i} \bar{\rho}_j
\]

(A.7)

with the notation as before.
We start by noting that
\[
\text{tr}_i \left( \bar{\rho}_{C_m} \prod_{j \in A_n \setminus C_m} \bar{\rho}_j \right) = \begin{cases} 
\bar{\rho}_{C_m} \prod_{j \in (A_n \setminus i) \setminus C_m} \bar{\rho}_j & i \not\in C_m \\
\bar{\rho}_{C_m \setminus i} \prod_{j \in A_n \setminus C_m} \bar{\rho}_j & i \in C_m 
\end{cases}
\] (A.8)

It then follows that we can write
\[
\sum_{m=2}^{n} (-1)^{n-m} \sum_{C_m \subseteq A_n} \text{tr}_i \left( \bar{\rho}_{C_m} \prod_{j \in A_n \setminus C_m} \bar{\rho}_j \right) = \sum_{\ell \in A_n \setminus i} \text{tr}_i (-1)^{n-2} \prod_{j \in A_n \setminus \{i, \ell\}} \bar{\rho}_j \\
+ \sum_{m=2}^{n-2} \sum_{C_m \subseteq (A_n \setminus i)} (-1)^m \text{tr}_i \left( \bar{\rho}_{C_m} \bar{\rho}_i - \bar{\rho}_{C_m \cup \{i\}} \right) \prod_{j \in (A_n \setminus i) \setminus C_m} \bar{\rho}_j \\
= \sum_{\ell \in A_n \setminus i} (-1)^{n-2} \prod_{j \in A_n \setminus \{i, \ell\}} \bar{\rho}_j \\
= (n-1)(-1)^{n-2} \prod_{j \in A_n \setminus \{i\}} \bar{\rho}_j 
\] (A.9)
so that
\[
\text{tr}_i \bar{\rho}_{C_A^n} = (n-1)(-1)^{n-2} \prod_{j \in A_n \setminus \{i\}} \bar{\rho}_j - (1)^n (n-1) \prod_{j \in A_n \setminus i} \bar{\rho}_j \\
= 0 
\] (A.10)
which is the result we wanted.
Appendix B

Derivation of Equations of Motion hierarchies

In the main text we simply quoted the results for the equations of motion, for both a general multipartite system, and also for an $N$-qubit system. Here we give the derivations of these results.

B.1 Equation of Motion for $N$-Partite system

Write begin by writing the Hamiltonian as a "free" single-system part, plus a pairwise interaction term, viz.,

$$ H = H^0 + H^I = \sum_j \left( H_j^0 + \frac{1}{2} \sum_{i \neq j} H_{ij}^I \right) $$  \hspace{1cm} (B.1)

The equation of motion is then

$$ i\partial_t \rho_S = [H, \rho_S] = \sum_{\mathcal{A} \subseteq S} \left[ H, \left( \prod_{j \notin \mathcal{A}} \tilde{\rho}_j \right) \tilde{\rho}_C^\mathcal{A} \right] $$

$$ = \sum_{j \in S} \left\{ \left[ H_j^0 + \sum_{j \neq i \in S} \frac{1}{2} H_{ij}^0, \left( \prod_{j \notin \mathcal{A}} \tilde{\rho}_j \right) \tilde{\rho}_C^\mathcal{A} \right] \right\} $$ \hspace{1cm} (B.2)

for the part of the above containing the non-interacting part of the Hamiltonian each $j$ is either in $\mathcal{A}$ or not $\mathcal{A}$, for the interacting part there are three possible situations (see figure [B.1]): Both $i, j \in \mathcal{A}$, only one of $i$ or $j$ in $\mathcal{A}$, and both $i, j \notin \mathcal{A}$. We can
Figure B.1: The different classes of interaction involving \( \mathcal{A} \). In (i) we have interactions entirely between cells inside \( \mathcal{A} \); in (ii) we have interactions between cells inside \( \mathcal{A} \) and cells outside; and in (iii) the interactions are entirely between cells outside \( \mathcal{A} \). The interactions are denoted by the wavy line.

split the sums up accordingly; one has

\[
\sum_{\mathcal{A}} \left[ H, \left( \prod_{j \notin \mathcal{A}} \bar{\rho}_j \right) \bar{\rho}_A^C \right] = \sum_{\mathcal{A} \subseteq \mathcal{S}} \left\{ \sum_{j \in \mathcal{A}} [H^0_j, \bar{\rho}_A^C] \prod_{i \notin \mathcal{A}} \bar{\rho}_i + \bar{\rho}_A^C \sum_{j \notin \mathcal{A}} [H^0_j, \bar{\rho}_j] \prod_{i \notin \mathcal{A} \cup \{j\}} \bar{\rho}_i \right. \\
+ \sum_{j \in \mathcal{A}} \sum_{i \notin \mathcal{A} \cup \{j\}} \left[ \frac{1}{2} H^I_{ij}, \bar{\rho}_A^C \right] \prod_{k \notin \mathcal{A}} \bar{\rho}_k + \sum_{j \notin \mathcal{A}} \sum_{i \notin \mathcal{A}} \left[ \frac{1}{2} H^I_{ij}, \bar{\rho}_A^C \bar{\rho}_i \right] \prod_{k \notin \mathcal{A} \cup \{i\}} \bar{\rho}_k \\
\left. + \bar{\rho}_A^C \sum_{j \notin \mathcal{A} \cup \{j\}} \sum_{i \notin \mathcal{A} \cup \{j\}} \left[ \frac{1}{2} H^I_{ij}, \bar{\rho}_j \bar{\rho}_i \right] \prod_{k \notin \mathcal{A} \cup \{i,j\}} \bar{\rho}_k \right\}. \tag{B.3}
\]

Now we trace out a set \( \mathcal{C} \) of cells. This gives

\[
\text{tr}_\mathcal{C} \left[ H, \sum_{\mathcal{A}} \bar{\rho}_A^C \prod_{i \notin \mathcal{A}} \bar{\rho}_i \right] = \sum_{\mathcal{A}} \text{tr}_\mathcal{C} \sum_{j \in \mathcal{A}} [H^0_j, \bar{\rho}_A^C] \prod_{i \notin \mathcal{A} \cup \{j\}} \bar{\rho}_i + \sum_{\mathcal{A}} \text{tr}_\mathcal{C} \bar{\rho}_A^C \sum_{j \notin \mathcal{A} \cup \{j\}} [H^0_j, \bar{\rho}_j] \prod_{i \notin \mathcal{A} \cup \{i\}} \bar{\rho}_i \\
+ \sum_{j \in \mathcal{A}} \sum_{i \notin \mathcal{A} \cup \{j\}} \text{tr}_\mathcal{C} \left[ \frac{1}{2} H^I_{ij}, \bar{\rho}_A^C \right] \prod_{k \notin \mathcal{A}} \bar{\rho}_k + \sum_{j \notin \mathcal{A}} \sum_{i \notin \mathcal{A}} \text{tr}_\mathcal{C} \left[ \frac{1}{2} H^I_{ij}, \bar{\rho}_A^C \bar{\rho}_i \right] \prod_{k \notin \mathcal{A} \cup \{i\}} \bar{\rho}_k \\
+ \bar{\rho}_A^C \sum_{j \notin \mathcal{A} \cup \{j\}} \sum_{i \notin \mathcal{A} \cup \{j\}} \text{tr}_\mathcal{C} \left[ \frac{1}{2} H^I_{ij}, \bar{\rho}_j \bar{\rho}_i \right] \prod_{k \notin \mathcal{A} \cup \{i,j\}} \bar{\rho}_k. \tag{B.4}
\]

Let us simplify each term in the above equation separately:

1. First consider the terms involving \( H^0_j \):

   (a) Consider the first sum in eqtn. \( \{B.4\} \), viz.,

   \[
   \sum_{\mathcal{A}} \text{tr}_\mathcal{C} \sum_{j \in \mathcal{A}} [H^0_j, \bar{\rho}_A^C] \prod_{i \notin \mathcal{A} \cup \{j\}} \bar{\rho}_i \tag{B.5}
   \]

   - The terms are trivially zero when the overlap \( \mathcal{C} \cap \mathcal{A} \neq \emptyset \) or \( \{j\} \).
   - If the overlap contains exactly one cell \( \mathcal{C} \cap \mathcal{A} = \{j\} \), then we have the following identity

     \[
     \text{tr}_j \left[ H^0_j, \bar{\rho}_A^C \right] = (H^0_j)_{mn}(\bar{\rho}_A^C)_{mm} - (H^0_j)_{nm}(\bar{\rho}_A^C)_{mn} = 0.
     \]
where $M$ is an index on the Hilbert space of states on the set of cells $A \setminus \{ j \}$ and $m, n$ are indices on the Hilbert space at $j$, and repeated indices are summed so $(\rho_A^{\mathcal{C}M})_{mn} = \sum_M (mM)(\rho_A^\mathcal{M})_{mn}^\mathcal{M}$. 

We see therefore that only terms with no overlap $\mathcal{C} \cap A = \emptyset$ contribute to the first sum in eqtn. (B.4):

$$
\sum_{\mathcal{C} \subseteq \mathcal{S}} \sum_{j \in A} \text{tr} \mathcal{C} \sum_{i \notin A} \left[ H_0^j, \bar{\rho}_A^\mathcal{C} \right] \prod_{i \notin A} \bar{\rho}_i = \sum_{\mathcal{C} \subseteq (\mathcal{S} \setminus \mathcal{C})} \sum_{j \in A} \left[ H_0^j, \bar{\rho}_A^\mathcal{C} \right] \prod_{i \notin A} \bar{\rho}_i \tag{B.6}
$$

(b) Consider now the second sum in (B.4), viz.,

$$
\text{tr} \mathcal{C} \sum_{j \notin A} \sum_{i \notin A \cup \{ j \}} N_{ij} \prod_{i \notin A \cup \{ j \}} \bar{\rho}_i \tag{B.8}
$$

The terms are zero when $A \cap \mathcal{C} \neq \emptyset$ and when $j \in \mathcal{C}$, so that

$$
\sum_{\mathcal{C} \subseteq \mathcal{S}} \sum_{i \notin A \cup \{ j \}} \text{tr} \mathcal{C} \sum_{j \notin A \cup \{ j \}} \left[ H_0^j, \bar{\rho}_j \right] \prod_{i \notin A \cup \{ j \}} \bar{\rho}_i = \sum_{\mathcal{C} \subseteq (\mathcal{S} \setminus \mathcal{C})} \sum_{j \notin A \cup \{ j \}} \left[ H_0^j, \bar{\rho}_j \right] \prod_{i \notin \mathcal{S} \setminus (\mathcal{A} \cup \mathcal{C})} \bar{\rho}_i \tag{B.7}
$$

The last line here requires a bit of thought; it reflects the fact that summing over all possible $\mathcal{A} \subseteq (\mathcal{S} \setminus \mathcal{C})$, then over $j \in (\mathcal{S} \setminus (\mathcal{C} \cup \mathcal{A}))$, is equivalent to summing over all possible $\mathcal{A} \subseteq (\mathcal{S} \setminus \mathcal{C})$ and all possible $j \in \mathcal{A}$.

2. Now consider the terms involving the interaction Hamiltonian $H_{ij}^I$.

(a) Consider first the third sum in equation (B.4), viz.,

$$
\sum_{\mathcal{A}} \sum_{j \in A} \sum_{i \in A \setminus \{ j \}} \text{tr} \mathcal{C} \left[ \frac{1}{2} H_{ij}^I, \bar{\rho}_A^\mathcal{C} \right] \prod_{k \notin A} \bar{\rho}_k \tag{B.8}
$$

which contains all the terms where cells inside $\mathcal{A}$ are interacting with each other, i.e., case (i) in figure [B.1].

- If the intersection $\mathcal{C} \cap \mathcal{A}$ contains cells other than $i$ or $j$, then

$$
\text{tr} \mathcal{C} \left[ \frac{1}{2} H_{ij}^I, \bar{\rho}_A^\mathcal{C} \right] \prod_{k \notin A} \bar{\rho}_k = 0.
$$
• If the intersection $C \cap A = \{i, j\}$ then

$$\text{tr}_C \left[ \frac{1}{2} H_{ij}, \bar{\rho}_A^C \right] \prod_{k \notin A} \bar{\rho}_k = 0.$$ 

so that there are only nonzero terms in the sum when the intersection $A \cap C$ contains exactly one or zero elements.

• If the intersection is one of $C \cap A = \{i\}$ or $\{j\}$ then

$$\text{tr}_C \left[ \frac{1}{2} H_{ij}, \bar{\rho}_A^C \right] \prod_{k \notin A} \bar{\rho}_k = \text{tr}_{\{i\}} \left( \frac{1}{2} H_{ij}, \bar{\rho}_A^C \right) \prod_{k \notin (A \cup \{i\})} \bar{\rho}_k$$

which is not necessarily zero.

• When both $i, j$ are in $A \setminus C$ then

$$\text{tr}_C \left[ \frac{1}{2} H_{ij}, \bar{\rho}_A^C \right] \prod_{k \notin A} \bar{\rho}_k = \text{tr}_{\{i\}} \left( \frac{1}{2} H_{ij}, \bar{\rho}_A^C \right) \prod_{k \notin (A \cup \{i\})} \bar{\rho}_k.$$ 

Thus there only two kinds of term in the sum (B.8) that matter. The first are those where both $i, j \notin C$ and $C \cap A$. The second are those where only one of $i$ or $j$ are in $C$ (say $i \in C$) and $A \cap C = \{i\}$. Thus

$$\sum_A \sum_{j \in A} \sum_{i \in A \setminus \{j\}} \text{tr}_C \left[ \frac{1}{2} H_{ij}, \bar{\rho}_A^C \right] \prod_{k \notin A} \bar{\rho}_k = \sum_{A \subseteq (S \setminus C)} \sum_{j \in A} \sum_{i \in A \setminus \{j\}} \text{tr}_C \left[ \frac{1}{2} H_{ij}, \bar{\rho}_A^C \right] \prod_{k \notin A} \bar{\rho}_k$$

$+ \sum_{A \subseteq S \setminus C} \sum_{j \in A} \text{tr}_C \left[ \frac{1}{2} H_{ij}, \bar{\rho}_A^C \right] \prod_{k \notin A} \bar{\rho}_k$

$$= \sum_{A \subseteq (S \setminus C)} \sum_{j \in A} \sum_{i \in A \setminus \{j\}} \text{tr}_C \left[ \frac{1}{2} H_{ij}, \bar{\rho}_A^C \right] \prod_{k \notin A \cup C} \bar{\rho}_k$$

$+ \sum_{A \subseteq (S \setminus C)} \sum_{i \in C} \sum_{j \in A} \text{tr}_C \left[ \frac{1}{2} H_{ij}, \bar{\rho}_A^C \right] \prod_{k \notin A \cup C} \bar{\rho}_k$  \hspace{1cm} (B.9)

(b) The fourth sum in eqtn. (B.4), viz.,

$$\sum_A \sum_{j \in A} \sum_{i \notin A} \text{tr}_C \left[ \frac{1}{2} H_{ij}, \bar{\rho}_A^C \bar{\rho}_i \right] \prod_{k \notin A \cup \{i\}} \bar{\rho}_k$$  \hspace{1cm} (B.10)

is a sum over terms involving interactions between $j$ in $A$ and $i$ not in $A$ (ie., terms like (ii) in figure B.1).

• When neither $i$ nor $j$ are in $C$, then

$$\text{tr}_C \left[ \frac{1}{2} H_{ij}, \bar{\rho}_A^C \bar{\rho}_i \right] \prod_{k \notin A \cup \{i\}} \bar{\rho}_k = \text{tr}_C \left[ \frac{1}{2} H_{ij}, \bar{\rho}_A^C \bar{\rho}_i \right] \prod_{k \notin (A \cup C \cup \{i\})} \bar{\rho}_k.$$
• When there is an overlap $A \cup C$ which contains an element other than $j$, then
  \[
  \text{tr} \left[ \frac{1}{2} H_{ij}, \rho_A^{C} \bar{\rho}_i \right] \prod_{k \notin A \cup \{i\}} \bar{\rho}_k = 0.
  \]

• When $i$ is in $C$ and $A \cap C = \emptyset$, then
  \[
  \text{tr} \left[ \frac{1}{2} H_{ij}, \rho_A^{C} \bar{\rho}_i \right] \prod_{k \notin A \cup \{i\}} \bar{\rho}_k = \left[ \frac{1}{2} \text{tr} (H_{ij} \bar{\rho}_i), \rho_A^{C} \right] \prod_{k \notin (A \cup C \cup \{i\})} \bar{\rho}_k.
  \]

• When $j$ is in $C$ but $i$ is not, then
  \[
  \text{tr} \left[ \frac{1}{2} H_{ij}, \rho_A^{C} \bar{\rho}_i \right] \prod_{k \notin A \cup \{i\}} \bar{\rho}_k = \text{tr} \left[ \frac{1}{2} H_{ij}, \rho_A^{C} \bar{\rho}_i \right] \prod_{k \notin (A \cup C \cup \{i\})} \bar{\rho}_k.
  \]

• If $i$ and $j$ are in $C$, then
  \[
  \text{tr} \left[ \frac{1}{2} H_{ij}, \rho_A^{C} \bar{\rho}_i \right] \prod_{k \notin A \cup \{i\}} \bar{\rho}_k = 0.
  \]

Thus the sum (B.10) is
\[
\sum_{A} \sum_{j \in A} \text{tr} \left[ \frac{1}{2} H_{ij}, \rho_A^{C} \bar{\rho}_i \right] \prod_{k \notin A \cup \{i\}} \bar{\rho}_k = \\
\sum_{A \subseteq (S \setminus C)} \sum_{j \in A} \sum_{i \notin (A \cup C)} \left[ \frac{1}{2} H_{ij}, \rho_A^{C} \bar{\rho}_i \right] \prod_{k \notin (A \cup C \cup \{i\})} \bar{\rho}_k + \\
\sum_{A \subseteq (S \setminus C)} \sum_{j \notin A} \sum_{i \in A} \left[ \frac{1}{2} \text{tr} (H_{ij} \bar{\rho}_i), \rho_A^{C} \right] \prod_{k \notin (A \cup C \cup \{i\})} \bar{\rho}_k + \\
\sum_{A \subseteq (S \setminus C)} \sum_{j \in A} \sum_{i \notin A} \left[ \frac{1}{2} \text{tr} (H_{ij} \bar{\rho}_i), \rho_A^{C} \bar{\rho}_i \right] \prod_{k \notin (A \cup C \cup \{i\})} \bar{\rho}_k
\]
(B.11)

(c) The fifth sum in eqtn. (B.4), viz.,
\[
\sum_{A} \text{tr} \rho_A^{C} \sum_{j \notin A} \sum_{i \notin A \cup \{j\}} \left[ \frac{1}{2} H_{ij}, \bar{\rho}_j \bar{\rho}_i \right] \prod_{k \notin A \cup \{i,j\}} \bar{\rho}_k
\]
(B.13)
is a sum over the interactions shown in figure (B.1) (iii), where both $i$ and $j$ are not in $C$. Then
• When \( i, j \in \mathcal{C} \), we have
\[
\text{tr}_{\mathcal{C}} \rho_A^C \left[ \frac{1}{2} H_{ij}, \tilde{\rho}_j \tilde{\rho}_i \right] \prod_{k \notin A \cup \{i,j\}} \tilde{\rho}_k = 0.
\]

• When \( \mathcal{A} \cap \mathcal{C} \neq \emptyset \), we have
\[
\text{tr}_{\mathcal{C}} \rho_A^C \left[ \frac{1}{2} H_{ij}, \tilde{\rho}_j \tilde{\rho}_i \right] \prod_{k \notin A \cup \{i,j\}} \tilde{\rho}_k = 0.
\]

• When one of \( i \) and \( j \) (say \( i \)) is in \( \mathcal{C} \) and the other is not, then (and \( \mathcal{A} \cap \mathcal{C} = \emptyset \))
\[
\text{tr}_{\mathcal{C}} \rho_A^C \left[ \frac{1}{2} H_{ij}, \tilde{\rho}_j \tilde{\rho}_i \right] \prod_{k \notin A \cup \{i,j\}} \tilde{\rho}_k = \rho_A^C \left[ \frac{1}{2} \text{tr}_i \left( H_{ij} \tilde{\rho}_i \right), \tilde{\rho}_j \right] \prod_{k \notin (A \cup \{j\} \cup \mathcal{C})} \tilde{\rho}_k.
\]

• When neither \( i \) nor \( j \) are in \( \mathcal{C} \) and \( \mathcal{A} \cap \mathcal{C} = \emptyset \), we have
\[
\text{tr}_{\mathcal{C}} \rho_A^C \left[ \frac{1}{2} H_{ij}, \tilde{\rho}_j \tilde{\rho}_i \right] \prod_{k \notin A \cup \{i,j\}} \tilde{\rho}_k = \rho_A^C \left[ \frac{1}{2} H_{ij}, \tilde{\rho}_j \tilde{\rho}_i \right] \prod_{k \notin A \cup \{i,j\} \cup \mathcal{C}} \tilde{\rho}_k.
\]

Thus the sum (B.13) is given by
\[
\sum_{\mathcal{A}} \text{tr}_{\mathcal{C}} \rho_A^C \sum_{j \notin A \cup \mathcal{A} \cup \{i\}} \prod_{k \notin (A \cup \{j\} \cup \mathcal{C})} \tilde{\rho}_k =
\sum_{\mathcal{A} \subseteq C} \sum_{i \in \mathcal{C}} \sum_{\mathcal{A} \notin \mathcal{C}} \rho_A^C \left[ \frac{1}{2} \text{tr}_i \left( H_{ij} \tilde{\rho}_i \right), \tilde{\rho}_j \right] \prod_{k \notin (A \cup \{j\} \cup \mathcal{C})} \tilde{\rho}_k
+ \sum_{\mathcal{A} \subseteq \mathcal{C}} \sum_{i \notin \mathcal{C}} \sum_{\mathcal{A} \notin \mathcal{C}} \rho_A^C \left[ \frac{1}{2} H_{ij}, \tilde{\rho}_j \tilde{\rho}_i \right] \prod_{k \notin A \cup \{i,j\} \cup \mathcal{C}} \tilde{\rho}_k.
\]

Thus finally, inserting equations (B.6), (B.7), (B.9), (B.12), and (B.14) into (B.4), we
have

\[
\text{tr}_C[H, \rho_S] = \sum_{\mathcal{A} \in S \setminus C} \left\{ \sum_{j \in \mathcal{A}} \left[ H_j^0, \rho_C^j \right] \prod_{i \in S \setminus (\mathcal{A} \cup \{j\})} \bar{\rho}_i \right. \\
+ \rho_A^C \sum_{i \in S \setminus (\mathcal{A} \cup \{j\})} \left[ H_i^0, \bar{\rho}_i \right] \prod_{j \in S \setminus (\mathcal{A} \cup \{i\})} \bar{\rho}_j \\
+ \sum_{j \in \mathcal{A}} \sum_{i \in \mathcal{A} \setminus \{j\}} \left[ \frac{1}{2} H_{ij}^C, \rho_C^j \right] \prod_{k \in S \setminus (\mathcal{A} \cup \{i, j\})} \bar{\rho}_k + \sum_{i \in \mathcal{C}} \sum_{j \in \mathcal{A}} \text{tr}_i \left[ H_{ij}^C, \rho_C^j \right] \prod_{k \in S \setminus (\mathcal{A} \cup \{i, j\})} \bar{\rho}_k \\
+ \rho_A^C \sum_{k \in S \setminus (\mathcal{A} \cup \{i\})} \sum_{l \in S \setminus (\mathcal{A} \cup \{k, l\})} \left[ H_{kl}^C, \bar{\rho}_k \right] \prod_{j \in S \setminus (\mathcal{A} \cup \{k, l\})} \bar{\rho}_j \\
+ \sum_{j \in \mathcal{A}} \sum_{i \in \mathcal{A} \setminus \{j\}} \left[ H_{ij}^C, \bar{\rho}_i \right] \prod_{k \in S \setminus (\mathcal{A} \cup \{i, j\})} \bar{\rho}_k \\
+ \sum_{l \in \mathcal{C}} \sum_{k \in \mathcal{A}} \text{tr}_l \left[ H_{lk}^C, \rho_C^j \right] \prod_{j \in S \setminus (\mathcal{A} \cup \{k\})} \bar{\rho}_j \\
+ \sum_{l \in \mathcal{C}} \sum_{k \in \mathcal{A}} \text{tr}_l \left[ H_{lk}^C, \rho_C^j \right] \prod_{j \in S \setminus (\mathcal{A} \cup \{k\})} \bar{\rho}_j \right\}. \tag{B.15}
\]

Comparing this with equation (B.3), we see that all of those terms above which do not contain an explicit trace can be collected to give \([H_{S \setminus C}, \bar{\rho}_{S \setminus C}]\), with

\[
H_{S \setminus C} = \sum_{j \in S \setminus C} \left( H_j^0 + \frac{1}{2} \sum_{j \in S \setminus (\mathcal{C} \cup \{j\})} H_{ij}^1 \right) \tag{B.16}
\]

so that

\[
i \partial_t \bar{\rho}_{S \setminus C} = [H_{S \setminus C}, \bar{\rho}_{S \setminus C}] + \mathcal{T} \tag{B.17}
\]
The extra “trace term" $TT$ is

$$TT = i \sum_{l \in C} \text{tr} \left\{ \sum_{A \subseteq (S \setminus C)} \sum_{i \in A} \left[ H_{il}^I, \tilde{\rho}_i^C \right] \tilde{\rho}_l + \left[ H_{il}^I, \rho_{(A \setminus \{l\})}^C \right] \prod_{j \in (S \setminus C) \setminus A} \tilde{\rho}_j \right\}$$

(B.18)

$$= i \sum_{l \in C} \text{tr} \left[ \sum_{i \in S \setminus C} H_{il}^I, \sum_{A \subseteq (S \setminus C) \cup \{l\}} \rho_{(S \setminus C) \cup \{l\}}^C \prod_{j \in ((S \setminus C) \cup \{l\}) \setminus A} \tilde{\rho}_j \right]$$

(B.19)

$$= \sum_{l \in C} \left[ \sum_{i \in S \setminus C} H_{il}^I, \tilde{\rho}_{(S \setminus C) \cup \{l\}} \right]$$

(B.20)

Thus, finally, we have the result

$$i \partial_t \tilde{\rho}_{S \setminus C} = [H_{S \setminus C}, \tilde{\rho}_{S \setminus C}] + i \sum_{l \in C} \left[ \sum_{i \in S \setminus C} H_{il}^I, \tilde{\rho}_{(S \setminus C) \cup \{l\}} \right].$$

(B.21)

If we now relabel the set $(S \setminus C) \rightarrow A$, we get the result (4.3) in the text.

### B.2 Equation of Motion for $N$-Qubit system

We now want to derive the equations of motion (4.7) for $N$-qubits. The Hamiltonian is

$$H = \sum_i \frac{1}{2} h_i \cdot \sigma_i + \sum_{i=1}^N \sum_{j<i} \frac{1}{2} V^\mu_\nu_{ij} \sigma_i^\mu \sigma_j^\nu$$

(B.22)

which we write as $H = H_0 + H_V$.

We wish to calculate

$$\frac{d}{dt} \left\langle \prod_{j \in C} \sigma_j^{\mu_j} \right\rangle = -i \left\langle \left[ H, \prod_{j \in C} \sigma_j^{\mu_j} \right] \right\rangle.$$

(B.23)

We thus need the commutators

$$\left[ H_0, \prod_{j \in C} \sigma_j^{\mu_j} \right] = \sum_{i \in C} \frac{1}{2} h_i^\lambda [\sigma_i^\lambda, \sigma_i^{\mu_i}] \prod_{j \in C \setminus \{i\}} \sigma_j^{\mu_j}$$

$$= i \sum_{i \in C} \varepsilon^{\mu_i \lambda \nu_i} h_i^\lambda \sigma_i^{\nu_i} \prod_{j \in C \setminus \{i\}} \sigma_j^{\mu_j}$$

(B.24)
and
\[
\left[ H_V, \prod_{j \in C} \sigma_j^{\mu_j} \right] = \sum_{i=1}^N \sum_{k<i} \frac{1}{2} V_{ik} \left[ \sigma_i^{\alpha} \sigma_k^{\beta}, \prod_{j \in C} \sigma_j^{\mu_j} \right] \tag{B.25}
\]

The commutator on the right of the previous expression is non zero when either one of \(i, k\) or both \(i\) and \(k\) are in \(C\). Consider the case when \(i\) is in \(C\) but \(k\) is not; then we have
\[
\left[ \sigma_i^{\alpha} \sigma_k^{\beta}, \prod_{j \in C} \sigma_j^{\mu_j} \right] = 2i \varepsilon_{\mu_i \alpha \nu_i} \sigma_i^{\nu_i} \sigma_k^{\beta} \prod_{j \in C \setminus i} \sigma_j^{\mu_j} \tag{B.26}
\]
On the other hand if both \(i\) and \(k\) are in \(C\), then we have
\[
\left[ \sigma_i^{\alpha} \sigma_k^{\beta}, \prod_{j \in C} \sigma_j^{\mu_j} \right] = \left[ \sigma_i^{\alpha} \sigma_k^{\beta}, \sigma_i^{\mu_i} \sigma_k^{\mu_k} \right] \prod_{j \in C \setminus \{i, k\}} \sigma_j^{\mu_j} = 2i \left( \varepsilon_{\mu_i \alpha \nu_i} \delta_{\mu_k \beta} \sigma_j^{\nu_j} + \varepsilon_{\mu_k \beta \nu_k} \sigma_k^{\nu_k} \delta_{\mu_j \alpha} \right) \prod_{j \in C \setminus \{i, k\}} \sigma_j^{\mu_j} \tag{B.27}
\]

Putting equations (B.26) and (B.26) into the equation of motion for the correlator (B.23) one gets the hierarchy of equations of motion,
\[
\frac{d}{dt} \left\langle \prod_{i \in A} \sigma_i^{\mu_i} \right\rangle = \sum_{i \in A} \varepsilon^{\mu_i \alpha \nu_i} h_i^{\alpha} \left\langle \prod_{j \in A \setminus \{i\}} \sigma_j^{\nu_j} \right\rangle + \sum_{i \in A} \sum_{j \not\in A} \varepsilon^{\mu_i \alpha \nu_i} V_{ij}^{\alpha \lambda} \left\langle \sigma_i^{\alpha} \sigma_j^{\nu_j} \prod_{k \in A \setminus \{i, j\}} \sigma_k^{\mu_k} \right\rangle \\
+ \sum_{i \in A} \sum_{j \in A \setminus \{i\}} \varepsilon^{\mu_i \alpha \nu_i} V_{ij}^{\alpha \mu_j} \left\langle \prod_{k \in A \setminus \{i, j\}} \sigma_k^{\mu_k} \right\rangle. \tag{B.28}
\]

which is the hierarchy of equations of motion for the spin correlators that we wished to derive (cf. eqtn. (4.7)).
Appendix C

Matrix Propagator for 2-Spin System

In the main text we worked out explicitly the equation of motion for the entanglement correlators of a simple 2-spin system, with the Hamiltonian

\[ H = \frac{1}{2} [\Delta_1 \tau^x + \Delta_2 \sigma^x + \omega \tau^z \sigma^z] \]  

and eigenvalues \( \epsilon_1, \epsilon_2 \) (compare eqtn. (4.40) et seq.).

Here we write out explicitly the propagators which appear in the block matrix \( G(z) \) (the result for \( G(t) \) then being given by Fourier transformation). We have

\[
\begin{align*}
g_{11}(z) &= \left( \frac{\omega^2 z}{2 \omega_{30}(z^2 + \omega_{30}^2)} + \frac{\omega^4}{2 \omega_{21}(z^2 + \omega_{21}^2)} + \left(1 - \frac{\omega^4}{\omega_{30}^2 \omega_{21}^2}\right) \frac{1}{z}\right) \hat{x}\hat{x} \\
&+ \frac{z}{2 \omega_{30} \omega_{21}} \left\{ \left(\frac{\omega_{20}^2 - \Delta_1^2}{z^2 + \omega_{10}^2} + \frac{\omega_{20}^2 - \Delta_2^2}{z^2 + \omega_{20}^2}\right) (\hat{y}\hat{y} + \hat{z}\hat{z}) - 2 \omega^2 \left(\frac{\hat{y}\hat{y}}{z^2 + \omega_{10}^2} + \frac{\hat{z}\hat{z}}{z^2 + \omega_{20}^2}\right)\right\} \\
&+ \frac{\hat{y}\hat{z} - \hat{z}\hat{y}}{4 \omega_{30} \omega_{20}} \left\{ [\omega_{21}(\Delta_1 + \Delta_2) - \omega_{30}(\Delta_1 - \Delta_2)] \frac{\omega_{10}^2}{z^2 + \omega_{10}^2} \\
&+ [\omega_{21}(\Delta_1 - \Delta_2) + \omega_{30}(\Delta_1 + \Delta_2)] \frac{\omega_{20}^2}{z^2 + \omega_{20}^2}\right\} \\
&\quad (C.2)
\end{align*}
\]

\[
\begin{align*}
g_{12}(z) &= \hat{x}\hat{x} \left( \frac{2 \Delta_1 \Delta_2 \omega^2}{\omega_{30}^2 \omega_{21}^2} + \frac{z \omega^2}{2} \left(\frac{1}{\omega_{30}(z^2 + \omega_{30}^2)} - \frac{1}{\omega_{21}(z^2 + \omega_{21}^2)}\right)\right) = g_{21}(z) \\
&\quad (C.3)
\end{align*}
\]
for the “small” matrix propagators, and

\[
g_{1p\nu\beta}^\mu = \left[ z(z^2 + \omega_1^2)(z^2 + \omega_2^2) \right]^{-1} \Delta_1 \omega \left( 2 \Delta_2 z \hat{x}^\mu \hat{z}_\nu \hat{y}_\beta + [z^2 + \Delta_1^2 - \Delta_2^2 + \omega^2] \hat{x}^\mu \hat{z}_\nu \hat{y}_\beta \\
- [z^2 + \Delta_1^2 + \Delta_2^2 + \omega^2] \hat{x}^\mu \hat{y}_\nu \hat{z}_\beta - \hat{x}^\mu \hat{y}_\nu \hat{z}_\beta + \hat{x}^\mu \hat{y}_\nu \hat{z}_\beta + \Delta_1 \Delta_2 \hat{z}^\mu \hat{x}_\nu \hat{y}_\beta + z \Delta_1 \hat{z}^\mu \hat{x}_\nu \hat{y}_\beta \\
+ \omega \frac{z \Delta_2 \hat{y}^\mu \hat{x}_\nu \hat{y}_\beta + z^2 \hat{y}^\mu \hat{x}_\nu \hat{z}_\beta + \Delta_1 \Delta_2 \hat{z}^\mu \hat{x}_\nu \hat{y}_\beta + z \Delta_1 \hat{z}^\mu \hat{x}_\nu \hat{y}_\beta}{z^2 \omega^2 + (z^2 + \Delta_1^2)(z^2 + \Delta_2^2)} \right]
\]

(C.5)

\[
g_{pp\nu\beta}^{\mu\alpha} = \frac{1}{z} \hat{x}^\mu \hat{x}^\alpha \hat{x}_\nu \hat{x}_\beta + \left[ (z^2 + \Delta_1^2)(z^2 + \Delta_2^2) + z^2 \omega^2 \right]^{-1} \left\{ z(z^2 + \Delta_1^2 + \omega^2) \hat{x}^\mu \hat{y}^\alpha \hat{x}_\nu \hat{y}_\beta \\
+ \Delta_2 (z^2 + \Delta_1^2) \left[ \hat{x}^\mu \hat{z}^\alpha \hat{x}_\nu \hat{y}_\beta - \hat{x}^\mu \hat{y}^\alpha \hat{x}_\nu \hat{z}_\beta \right] + z(z^2 + \Delta_1^2) \hat{x}^\mu \hat{z}^\alpha \hat{x}_\nu \hat{z}_\beta \\
+ z(z^2 + \Delta_2^2 + \omega^2) \left[ \hat{y}^\mu \hat{z}^\alpha \hat{x}_\nu \hat{y}_\beta + \Delta_1 (z^2 + \Delta_2^2) \left[ \hat{z}^\mu \hat{y}^\alpha \hat{x}_\nu \hat{y}_\beta - \hat{y}^\mu \hat{z}^\alpha \hat{x}_\nu \hat{y}_\beta \right] \\
+ z(z^2 + \Delta_2^2) \hat{z}^\mu \hat{z}^\alpha \hat{x}_\nu \hat{x}_\beta \right\} + (z^2 + \omega_2^2)^{-1} (z^2 + \omega_3^2)^{-1} \left\{ (z^2 + \Delta_1^2 + \Delta_2^2 + \omega^2) \left[ \left( \frac{\omega}{z} \right) \left( \hat{y}^\mu \hat{y}^\alpha \hat{y}_\nu \hat{y}_\beta + \hat{z}^\mu \hat{z}^\alpha \hat{z}_\nu \hat{z}_\beta \right) + z \left( \hat{y}^\mu \hat{z}^\alpha \hat{y}_\nu \hat{z}_\beta + \hat{z}^\mu \hat{y}^\alpha \hat{z}_\nu \hat{y}_\beta \right) \right] \\
+ \Delta_2^2 (z^2 - \Delta_1^2 + \Delta_2^2 + \omega^2) \left[ \hat{y}^\mu \hat{z}^\alpha \hat{y}_\nu \hat{y}_\beta - \hat{y}^\mu \hat{y}^\alpha \hat{y}_\nu \hat{z}_\beta + \hat{z}^\mu \hat{z}^\alpha \hat{z}_\nu \hat{y}_\beta - \hat{z}^\mu \hat{y}^\alpha \hat{z}_\nu \hat{z}_\beta \right] + \Delta_1 (z^2 + \Delta_1^2 - \Delta_2^2 + \omega^2) \left[ \hat{z}^\mu \hat{y}^\alpha \hat{y}_\nu \hat{y}_\beta + \hat{z}^\mu \hat{z}^\alpha \hat{y}_\nu \hat{y}_\beta - \hat{y}^\mu \hat{y}^\alpha \hat{y}_\nu \hat{z}_\beta - \hat{y}^\mu \hat{y}^\alpha \hat{z}_\nu \hat{z}_\beta \right] \\
+ 2 \Delta_1 \Delta_2 (z^2 + \omega^2) \left[ \hat{y}^\mu \hat{z}^\alpha \hat{y}_\nu \hat{z}_\beta - \hat{z}^\mu \hat{z}^\alpha \hat{z}_\nu \hat{y}_\beta \right] + 2 z \Delta_1 \Delta_2 \left[ \hat{y}^\mu \hat{z}^\alpha \hat{z}_\nu \hat{y}_\beta - \hat{z}^\mu \hat{y}^\alpha \hat{y}_\nu \hat{z}_\beta \right] \right\} \right.
\]

(C.6)

for the “large” matrix propagators. In these equations \( \hat{x} \), \( \hat{y} \), and \( \hat{z} \) are unit Cartesian vectors, and \( \hat{z} \) should not be confused with the complex frequency \( z \).

Formulae for \( g_{22} \), \( g_{21} \), and \( g_{2p} \), can be obtained from the expressions for \( g_{11} \), \( g_{21} \), and \( g_{1p} \), if we make the replacements \( \Delta_1 \rightarrow \Delta_2 \) and \( \Delta_2 \rightarrow \Delta_1 \) and adjust the tensor indices accordingly (\( \mu \rightarrow \alpha \), \( \nu \rightarrow \beta \), \( \alpha \rightarrow \mu \), \( \beta \rightarrow \nu \)). \( g_{p1}(z) \) and \( g_{p2}(z) \) can be obtained from \( g_{1p}, g_{2p} \) using the identities \( g_{p1}(z) = g_{1p}^T(-z) \) and \( g_{p2}(z) = g_{2p}^T(-z) \) (we have obtained these identities by examining the full solution).
Appendix D

Numerical Calculation of Single Spin Evolution in a Time Dependent Field.

Numerically integrating the equation of motion with a time dependent bias (6.42) can cause troubles. Using an ineffective time integration scheme (e.g., Runge-Kutta) one finds that the length of the qubit polarisation $|\langle \tau(t) \rangle|$ drifts over time even though it is an exact constant of motion. To fix this one must use an integrator that explicitly conserves the polarisation. The simplest such integrator based on the trotter product formula. We derive this integrator as follows, begin by writing the formal solution to the equations of motion as at time $t_{n+1}$ in terms of $\langle \tau(t_{n}) \rangle$ at an earlier time $t_{1}$ using a time ordered exponential,

$$\langle \tau(t_{n+1}) \rangle = \mathcal{T} \exp \left\{ \int_{t_{n}}^{t_{n+1}} dt' \left[ \Delta + \xi(t') \right] \right\} \langle \tau(t_{n}) \rangle. \quad (D.1)$$

Where $\mathcal{T}$ is the time ordering operator and the matrices $\xi(t)$ and $\Delta$ are

$$\Delta = \Delta_0 \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix} \quad (D.2)$$

$$\xi(t) = \xi(t) \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \quad (D.3)$$

Write $\delta t = t_{n+1} - t_{n}$ then we can expand the time ordered exponential using the Trotter product formula

$$\mathcal{T} \exp \left\{ \int_{t_{n}}^{t} dt' \left[ \Delta + \xi(t') \right] \right\} = \exp (\delta t \Delta) \exp \left( \int_{t_{n}}^{t} dt' \xi(t') \right) + \mathcal{O}(\delta t^2 \Delta^2, \delta t^2 \xi(t_{n})^2, \delta t^3 \xi''(t_{n})) \quad (D.4)$$

$$\quad = \exp (\delta t \Delta) \exp (\delta t \xi(t_{n})) + \mathcal{O}(\delta t^2 \Delta^2, \delta t^2 \xi(t_{n})^2, \delta t^3 \xi''(t_{n})). \quad (D.5)$$

Note the error estimates above assume that $\xi(t)$ is sufficiently smooth, in the particular case where $\xi(t)$ is white noise with standard deviation $\lambda$ the last error estimate
becomes $O(\lambda \xi(t_n) \delta t^{3/2})$. Thus we can numerically integrate the equations of motion by setting $\delta t$ sufficiently small and iterating the following,

$$\langle \tau(t_{n+1}) \rangle = \exp(\delta t \Delta) \exp(\delta t \xi(t_n)) \langle \tau(t_n) \rangle$$  \hspace{1cm} (D.6)

with $t_n = n \delta t$. Because the matrices $\xi(t_n)$ and $\Delta$ are antisymmetric both of the matrix exponentials in (D.6) are orthogonal and each time step explicitly conserves the length of the polarisation vector.

### D.1 Treatment of Stochastic Forces

One can treat stochastic terms in the Hamiltonian numerically using the well developed theory of stochastic differential equations [39]. The diffusing bias $\xi(t)$ discussed in section 6.3.2 can be approximated, for a single realisation of the noise as follows. A set of random variables $\{r_i\}$ are drawn from a Gaussian distribution with mean zero and variance of one, one for each time step. Then the integral of the bias over the $n^{th}$ time step can be approximated by ($\xi_0$ is the initial value for the bias)

$$\int_{t_n}^{t_{n+\delta t_n}} ds \xi(s) \approx \xi_0 \delta t + \delta t \frac{3}{2} \Lambda_3^2 \sum_{j=0}^{n} r_j \equiv \delta \theta_n.$$  \hspace{1cm} (D.7)

With this the solution to the equation of motion can then be obtained iteratively using a modified version of equation (D.6)

$$\langle \tau(t_{n+1}) \rangle = \exp(\delta t \Delta) \exp \left[ \delta \theta_n \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \right] \langle \tau(t_n) \rangle.$$  \hspace{1cm} (D.8)

Then averages over $\xi$ can be computed by averaging over many different realisations for the $\{r_i\}$ variables.
Appendix E

Details of precessional decoherence calculations:

In this appendix we show the details omitted in section 7.2.

In section E.1 show how to generalise the result derived in 7.2.3 for the return probability of the central spin, to get the full reduced density matrix for the central spin. In section E.2 we calculate the next-to leading order correction to $\langle \tau^+ \rangle$ discussed in section 7.68. Then in section E.3 we calculate correlators of the central spin with the spin bath, deriving the results presented in section 7.2.4.
E.1 Calculating the full reduced density matrix for the central spin.

Calculating the full reduced density matrix from section 7.2.3. Write the equations (7.40-7.51) as follows

\[ A^{(n)}_+ = \frac{1}{2^n} \sum_{\ell=0}^n \binom{2n}{2\ell} a^{(n\ell)}_{+-} \]  
\[ A^{(n)}_{++} = -\frac{1}{2^n} \sum_{\ell=0}^{n-1} \binom{2n}{2\ell+1} a^{(n\ell)}_{++} \]  
\[ A^{(n)}_{+\uparrow} = \frac{1}{2^{n+1}} \sum_{\ell=0}^n \binom{2n+1}{2\ell} a^{(n\ell)}_{+\uparrow} \]  
\[ A^{(n)}_{-\downarrow} = -\frac{1}{2^n} \sum_{\ell=0}^n \binom{2n}{2\ell+1} a^{(n\ell)}_{-\downarrow} \]  
\[ A^{(n)}_{\uparrow\uparrow} = \frac{1}{2^n} \sum_{\ell=0}^{n-1} \binom{2n}{2\ell} a^{(n\ell)}_{\uparrow\uparrow} \]  
\[ A^{(n)}_{\downarrow\downarrow} = -\frac{1}{2^n} \sum_{\ell=0}^{n-1} \binom{2n}{2\ell} a^{(n\ell)}_{\downarrow\downarrow} \]  
\[ A^{(n)}_{-\uparrow} = -\frac{1}{2^n} \sum_{\ell=0}^n \binom{2n}{2\ell+1} a^{(n\ell)}_{-\uparrow} \]  
\[ A^{(n)}_{\uparrow\downarrow} = \frac{1}{2^n} \sum_{\ell=0}^n \binom{2n}{2\ell+1} a^{(n\ell)}_{\uparrow\downarrow} \]  

So the variables \( a^{(n\ell)}_{ab} \) for appropriate \( a, b \in \{a, +, -, \uparrow, \downarrow\} \) appearing in equations (E.1-E.12) are expectations of strings of operators appearing in equations (7.40-7.51). Using the same manipulations leading up to equation (7.58) the \( a^{(n\ell)}_{ab} \) coefficients can be written in the following form

\[ a^{(n\ell)}_{ab} = \int_0^{2\pi} \frac{d^n \xi}{(2\pi)^n} \exp \left\{ -n_{ab} N \beta^2 - N \beta^2 \sum_{q=1}^{n_{ab}-1} \sum_{q'=q}^{n_{ab}} \sum_{q''} \sum_{q'''} (c_{ab})_{qq'} \cos \left( 2 \sum_{q''=q+1}^{q'} \xi_q \right) \right\} . \]  

(E.13)
Table E.1: Parameters used in the transition expansion calculation of the reduced density matrix.

<table>
<thead>
<tr>
<th>a</th>
<th>b</th>
<th>$\gamma_{ab}$</th>
<th>$\tilde{\ell}_{ab}$</th>
<th>$n_{ab}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>+</td>
<td>-</td>
<td>$1$</td>
<td>$\ell$</td>
<td>$2n$</td>
</tr>
<tr>
<td>+</td>
<td>+</td>
<td>$-1$</td>
<td>$\ell + 1$</td>
<td>$2n$</td>
</tr>
<tr>
<td>+</td>
<td>↑</td>
<td>$1$</td>
<td>$\ell$</td>
<td>$2n + 1$</td>
</tr>
<tr>
<td>+</td>
<td>↓</td>
<td>$-1$</td>
<td>$\ell + 1$</td>
<td>$2n + 1$</td>
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<tr>
<td>-</td>
<td>-</td>
<td>$-1$</td>
<td>$\ell$</td>
<td>$2n$</td>
</tr>
<tr>
<td>-</td>
<td>+</td>
<td>$1$</td>
<td>$\ell + 1$</td>
<td>$2n$</td>
</tr>
<tr>
<td>-</td>
<td>↓</td>
<td>$-1$</td>
<td>$\ell$</td>
<td>$2n + 1$</td>
</tr>
<tr>
<td>-</td>
<td>↑</td>
<td>$1$</td>
<td>$\ell + 1$</td>
<td>$2n + 1$</td>
</tr>
<tr>
<td>$z$</td>
<td>↑</td>
<td>$1$</td>
<td>$0$</td>
<td>$2n$</td>
</tr>
<tr>
<td>$z$</td>
<td>↓</td>
<td>$-1$</td>
<td>$0$</td>
<td>$2n$</td>
</tr>
<tr>
<td>$z$</td>
<td>+</td>
<td>$1$</td>
<td>$0$</td>
<td>$2n + 1$</td>
</tr>
<tr>
<td>$z$</td>
<td>−</td>
<td>$-1$</td>
<td>$0$</td>
<td>$2n + 1$</td>
</tr>
</tbody>
</table>

The variables $(c_{ab})_{qq'}^n$ are of the form (note $q' > q$ in all terms)

$$(c_{ab})_{qq'}^n = \begin{cases} 
\gamma_{ab}(-1)^{q+q'} & \text{for } q > \tilde{\ell}_{ab} \text{ or } q' \leq \tilde{\ell}_{ab} \\
-\gamma_{ab}(-1)^{q+q'} & \text{for } q \leq \tilde{\ell}_{ab} \text{ and } q' > \tilde{\ell}_{ab}
\end{cases} \quad (E.14)$$

and the parameters $\gamma_{ab}$, $\tilde{\ell}_{ab}$, and $n_{ab}$ which appear in these expressions are given in the table E.1. Then by substituting

$$\chi_q = 2 \sum_{q'=1}^{q} \xi_{q'} + q\pi + \pi \left[ \Theta(q - \ell + \epsilon) + \Theta(-\gamma_{ab}) \right] \quad (E.15)$$

we get

$$a_{ab}^{(n\ell)} = \int_{0}^{2\pi} \frac{d^{\ell} \chi_{ab}}{(2\pi)^{n_{ab}}} \exp \left\{ -n_{ab}N\beta^2 - N2\beta^2 \sum_{q=1}^{2n_{ab}-1} \sum_{q'=q}^{n_{ab}} \cos (\chi_q - \chi_{q'}) \right\} \quad (E.16)$$

and the same set of steps that leads to (7.64) gives

$$a_{ab}^{(n\ell)} = \int_{0}^{\infty} dX Xe^{-\frac{X^2}{4\xi^2}} J_0(X)^{n_{ab}}. \quad (E.17)$$
Plugging this into equations (E.1-eq:lastAap), gives

\[ A^{(n)}_{+ -} \equiv \int dXP(X) \frac{1}{2^{2n}} \sum_{\ell=0}^{n} \left( \frac{2n}{2\ell + 1} \right) [J_0(X)]^{2n} \]  
(E.18)

\[ A^{(n)}_{+ +} \equiv -\int dXP(X) \frac{1}{2^{2n}} \sum_{\ell=0}^{n-1} \left( \frac{2n}{2\ell + 1} \right) [J_0(X)]^{2n+2} \]  
(E.19)

\[ A^{(n)}_{+ \uparrow} \equiv \int dXP(X) \frac{1}{2^{2n+1}} \sum_{\ell=0}^{n} \left( \frac{2n + 1}{2\ell + 1} \right) [J_0(X)]^{2n+1} \]  
(E.20)

\[ A^{(n)}_{+ \downarrow} \equiv -\int dXP(X) \frac{1}{2^{2n+1}} \sum_{\ell=0}^{n} \left( \frac{2n + 1}{2\ell + 1} \right) [J_0(X)]^{2n+1} \]  
(E.21)

\[ A^{(n)}_{- -} \equiv \int dXP(X) \frac{1}{2^{2n}} \sum_{\ell=0}^{n} \left( \frac{2n}{2\ell + 1} \right) [J_0(X)]^{2n} \]  
(E.22)

\[ A^{(n)}_{- +} \equiv -\int dXP(X) \frac{1}{2^{2n+1}} \sum_{\ell=0}^{n} \left( \frac{2n + 1}{2\ell + 1} \right) [J_0(X)]^{2n+2} \]  
(E.23)

\[ A^{(n)}_{- \uparrow} \equiv \int dXP(X) \frac{1}{2^{2n+1}} \sum_{\ell=0}^{n} \left( \frac{2n + 1}{2\ell + 1} \right) [J_0(X)]^{2n+1} \]  
(E.24)

\[ A^{(n)}_{- \downarrow} \equiv -\int dXP(X) \frac{1}{2^{2n+1}} \sum_{\ell=0}^{n} \left( \frac{2n + 1}{2\ell + 1} \right) [J_0(X)]^{2n+1} \]  
(E.25)

\[ A^{(n)}_{\uparrow \downarrow} \equiv \int dXP(X) \frac{1}{\frac{1}{2}} [J_0(X)]^{2n} \]  
(E.26)

\[ A^{(n)}_{\uparrow \uparrow} \equiv -\int dXP(X) \frac{1}{\frac{1}{2}} [J_0(X)]^{2n} \]  
(E.27)

\[ A^{(n)}_{\downarrow \downarrow} \equiv \int dXP(X) \frac{1}{\frac{1}{2}} [J_0(X)]^{2n+1} \]  
(E.28)

\[ A^{(n)}_{\downarrow \uparrow} \equiv -\int dXP(X) \frac{1}{\frac{1}{2}} [J_0(X)]^{2n+1} \]  
(E.29)

Plugging equations (E.18-E.29) into equations (7.37-7.37), gives the desired result, the same expansion one would have for an isolated qubit under the influence of the Hamiltonian \( H_0 = \frac{1}{2} \Delta_0 J_0(X) \tau^x \) averaged over the variable \( X \).

E.2 Next to leading order contributions to \( \langle \tau^x(t) \rangle \)

As discussed in section 7.68 we show the ext to leading order contributions to \( \langle \tau^x(t) \rangle \) is zero. We compute the next to leading order contribution to \( \langle \tau^\uparrow(t) \rangle \) from an initial density from the initial central spin density matrix \( | \uparrow \rangle \langle \downarrow | \) and show that this is zero. Then we will explain why this generalises to all next to leading order contributions.
to $\langle \tau^x(t) \rangle$.

\[
\delta \langle \tau^+(t) \rangle = \sum_{n=0}^{\infty} (-i\Delta_0)^{2n} \sum_{\ell=1}^{n} (-1)^\ell \int_0^t \{ \mathcal{D} \eta(t) \}^{2\ell} \int_0^t \{ \mathcal{D} \eta(t) \}^{2n-2\ell} \sum_{M=-N \neq 0}^{N} \left\{ \left( \prod_{q=1}^{\ell} \mathcal{P}_0 U^{(-1)^{q+1}} \right) \left[ \mathcal{P}_0 U^{(-1)^{p+1}} \mathcal{P}_M U^{(-1)^{p+2}} \right] \cdot \left( \prod_{q=p+2}^{2\ell} \mathcal{P}_0 U^{(-1)^{q+1}} \right) \left( \prod_{q=2\ell+1}^{2n} \mathcal{P}_0 U^{(-1)^{q}} \right) e^{i(1-1)^p/2 - \omega_0 M (t_p - t_{p+1})} \right. \\
+ \sum_{p=2\ell+1}^{2n-1} \left( \prod_{q=1}^{\ell} \mathcal{P}_0 U^{(-1)^{q+1}} \right) \left( \prod_{q=2\ell+1}^{p-1} \mathcal{P}_0 U^{(-1)^{q}} \right) \left[ \mathcal{P}_0 U^{(-1)^p} \mathcal{P}_M U^{(-1)^{p+1}} \right] \cdot \left( \prod_{q=p+2}^{2n} \mathcal{P}_0 U^{(-1)^{q}} \right) e^{i(1-1)^{p+1}/2 - \omega_0 M (t_{p-1} - t_{p+1})} \right\} 
\]

Here

\[
\int_0^t \{ \mathcal{D} \eta(t) \}^{2\ell} = \int_0^t dt_1 \int_0^{t_2} dt_2 \cdots \int_0^{t_{2\ell-1}} dt_{2\ell-1} \int_0^{t_2} dt_1 
\]

and we have used the following convention for non-commutative products

\[
\prod_{i=1}^{n} \hat{A}_i \equiv \hat{A}_1 \hat{A}_2 \hat{A}_3 \cdots \hat{A}_n. 
\]

Equation (E.30) consists of sums over the contributions from different paths for the central spin where the $p$'th tunneling event for the central spin is accompanied by a jump of bath $z$ magnetisation from zero to any possible value $M$ then back in the following central spin tunneling event. Now we calculate time integrations occurring in (E.30) using the identity

\[
\int_0^{t_1} dt_{p-1} \cdots \int_0^{t_2} dt_1 = \frac{t_p^{p-1}}{(p-1)!} 
\]
so that
\[
\int_0^t dt_2 \ldots \int_0^{t_{p+1}} dt_p \int_0^{t_p} dt_{p-1} \ldots \int_0^{t_2} dt_1 e^{-\frac{i(-1)^p}{2} \omega_0 M (t_p - t_{p+1})}
\]
\[
\int_0^t dt_n \ldots \int_0^{t_{p+1}} dt_p \frac{t_p^{p-1}}{(p-1)!} e^{-\frac{i(-1)^p}{2} \omega_0 M (t_p - t_{p+1})}
\]
\[
\int_0^t dt_2 \ldots \int_0^{t_{p+2}} dt_{p+1} \frac{1}{(p-1)!} e^{-\frac{i(-1)^p}{2} \omega_0 M t_{p+1}}
\]
\[
\int_0^t dt_2 \ldots \int_0^{t_{p+2}} dt_{p+1} \frac{1}{(p-1)!} e^{-\frac{i(-1)^p}{2} \omega_0 M t_{p+1}}
\]
\[
\sim \int_0^t dt_2 \ldots \int_0^{t_{p+2}} dt_{p+1} \frac{1}{(p-1)!} e^{-\frac{i(-1)^p}{2} \omega_0 M t_{p+1}}
\]
\[
\sim \frac{(1)^{p+1}}{M \omega_0} \int_0^t dt_2 \ldots \int_0^{t_{p+2}} dt_{p+1} \frac{1}{(p-1)!} t_{p+1}^{p-1}
\]
\[
\sim \frac{(1)^{p+1}}{M \omega_0} \int_0^t dt_2 \ldots \int_0^{t_{p+2}} dt_{p+1} \frac{1}{(p-1)!} t_{p+1}^{p-1}
\]
where we have kept the leading order secular terms. Thus the contribution \([E.30]\) becomes
\[
\delta \langle \tau^+ (t) \rangle \]
\[
\sum_{n=0}^{\infty} (-i \Delta_0)^{2n} \sum_{\ell=1}^{n} (-1)^{\ell} \sum_{M=-N \neq 0}^{N} \frac{i \ell^{2n-1}}{(2\ell)! (2n - 2\ell)! M \omega_0} \left\{ \sum_{p=1}^{2\ell-1} (-1)^{p+1} 2\ell \left( \prod_{q=1}^{p-1} \Psi_0 U(-1)^{q+1} \right) \right. \left[ \Psi_0 U(-1)^{p+1} \Psi_M U(-1)^{p+2} \right] \left( \prod_{q=p+2}^{2\ell} \Psi_0 U(-1)^{q+1} \right) \right.
\]
\[
\left. \cdot \left( \prod_{q=2\ell+1}^{2n} \Psi_0 U(-1)^q \right) \right\}
\]
\[
+ \sum_{p=2\ell+1}^{2n-1} \sum_{q=2\ell+1}^{2n} (-1)^p (2n - 2\ell) \left( \prod_{q=1}^{2\ell} \Psi_0 U(-1)^{q+1} \right) \left( \prod_{q=p+2}^{2\ell} \Psi_0 U(-1)^q \right) \left[ \Psi_0 U(-1)^p \Psi_M U(-1)^{p+1} \right]
\]
\[
\cdot \left( \prod_{q=p+2}^{2n} \Psi_0 U(-1)^q \right) \right\}.
\]
Now the terms in curly brackets in equation (E.35) only depend on the magnitude of $M$, this is because the terms containing $M$ are expectations of strings of projection operators sandwiching rotation matrices $U$, the unitary can be written

$$U^{(-1)^q} = \sum_{C \subseteq \mathcal{B}} (\prod_{i \in C} (-1)^q i \sin \beta_i (\sigma_i^+ + \sigma_i^-)) \prod_{j \not\in C} \cos \beta_i.$$  

(E.36)

Which depends on the raising operator and the lowering operator in the same way so that the terms where this string of operators specifies a jump to the manifold of states with magnetisation $+M$ will have the same amplitude as that where there is a jump to the manifold of states with magnetisation $-M$. Therefore the $+M$ and $-M$ terms in the sum (E.35) cancel exactly. This same set of statements is going to be true for any string of operators generated by the next to leading order orthogonality blocking approximation to the transition expansion of $\bar{\rho}_S$.

### E.3 Calculating correlators between bath and central spins.

Our goal here is to calculate various correlators given in section 7.2.4 between the central spin and up to two other spins. As discussed in the text only correlatives of operators which preserve the bath magnetisation are non zero in the orthogonality blocking approximation. Therefore the only applicable bath operators are,

$$\sigma_i^x \sigma_j^x = \sigma_i^+ \sigma_j^+ + \sigma_i^- \sigma_j^- + \sigma_i^+ \sigma_j^- + \sigma_i^- \sigma_j^+$$  

(E.37)

$$\sigma_i^y \sigma_j^y = -i\sigma_i^+ \sigma_j^- + i\sigma_i^- \sigma_j^+ + i\sigma_i^+ \sigma_j^- + i\sigma_i^- \sigma_j^+$$  

(E.38)

$$\sigma_i^z \sigma_j^z = -\sigma_i^+ \sigma_j^- + \sigma_i^- \sigma_j^+$$  

(E.39)

We will show later in section E.3.2 that, to leading order the correlators of the form $\langle \tau^x \sigma_i^z \rangle$ and $\langle \tau^y \sigma_i^z \sigma_j^z \rangle$ are to leading order,

$$\langle \tau^x \sigma_i^z \rangle (t) = \eta_i \langle \tau^x \rangle$$  

(E.42)

$$\langle \tau^y \sigma_i^z \sigma_j^z \rangle (t) = \eta_i \eta_j \langle \tau^y \rangle,$$  

(E.43)

where $\bar{\rho}_i(0) = |\eta_i\rangle \langle \eta_i|$. First we focus on the correlators between the central spin and the operators (E.37-E.37), which involve transverse components of the bath spins.

#### E.3.1 Correlators Involving Transverse Components of the Bath Spins

We begin by computing the contribution to $\langle | \uparrow \rangle \langle \uparrow | \sigma_i^+ \sigma_j^- \rangle (t)$ from the initial central spin density matrix $\bar{\rho}_S(0) = | \uparrow \rangle \langle \uparrow |$. 


In the leading order orthogonality blocking approximation the operator \( \langle \uparrow \uparrow | \sigma_i^+ \sigma_j^- \rangle \) ends up sandwiched between two \( \Phi_0 \) operators, so we have

\[
\langle \uparrow \uparrow | \sigma_i^+ \sigma_j^- \rangle (t) \approx \sum_{n=0}^{\infty} \left( -\frac{i\Delta_0}{2} \right)^{2n} \sum_{\ell=0}^{n} \int \{D\eta\}^{2\ell} \int \{D\eta\}^{2n-2\ell} \frac{d^{2n} \xi}{(2\pi)^{2n}} \cdot \exp \left\{ -n\beta^2 (N - 2) - (N - 1)\beta^2 \sum_{\ell' = 1}^{2n-1} \sum_{\ell'' = \ell'} (-1)^{\ell' + \ell''} \cos \left( 2 \sum_{q=\ell''+1}^{\ell'} \xi_q \right) \right\} \cdot \langle \prod_{q=1}^{2\ell} \left( e^{i\xi_q (\sigma_i^+ + \sigma_j^+)} e^{i(-1)^{q+1} \beta (\sigma_i^+ + \sigma_j^+)} \right) (\sigma_i^+ \sigma_j^-) \rangle 
\]

\[ \quad \cdot \prod_{q=2\ell+1}^{2n} \left( e^{i\xi_q (\sigma_i^+ + \sigma_j^+)} e^{i(-1)^{q+1} \beta (\sigma_i^+ + \sigma_j^+)} \right). \]  

(E.44)

(E.45)

Then using the usual maneuvers we have, the most secular terms in the transition expansion

\[
\langle \uparrow \uparrow | \sigma_i^+ \sigma_j^- \rangle (t) \approx \sum_{n=0}^{\infty} \left( -\frac{i\Delta_0}{2} \right)^{2n} \sum_{\ell=0}^{n} \frac{1}{(2\ell)! (2n - 2\ell)!} \int \frac{d^{2n} \xi}{(2\pi)^{2n}} \cdot \exp \left\{ -n\beta^2 (N - 2) - (N - 1)\beta^2 \sum_{\ell' = 1}^{2n-1} \sum_{\ell'' = \ell'} (-1)^{\ell' + \ell''} \cos \left( 2 \sum_{q=\ell''+1}^{\ell'} \xi_q \right) \right\} \cdot \langle \prod_{q=1}^{2\ell} \left( e^{i\xi_q (\sigma_i^+ + \sigma_j^+)} e^{i(-1)^{q+1} \beta (\sigma_i^+ + \sigma_j^+)} \right) (\sigma_i^+ \sigma_j^-) \rangle 
\]

\[ \quad \cdot \prod_{q=2\ell+1}^{2n} \left( e^{i\xi_q (\sigma_i^+ + \sigma_j^+)} e^{i(-1)^{q+1} \beta (\sigma_i^+ + \sigma_j^+)} \right). \]  

(E.46)

Obviously this expression depends on whether spins \( i \) and \( j \) are initially up or down, now we consider the different possibilities. Firstly We only need to evaluate the correlators involving bath spins \( i \) and \( j \) (the rest we have done in the previous
sections). These take the following possible values

\[ \langle \uparrow \mid \prod_{q=1}^{2\ell} \left( e^{i\xi_q \sigma^z} e^{i(-1)^{q+1} \beta \sigma^x} \right) \sigma^+_i \prod_{q=2\ell+1}^{2n} \left( e^{i\xi_q \sigma^z} e^{i(-1)^{q+1} \beta \sigma^x} \right) \mid \uparrow \rangle \]  

(E.47)

\[ \approx \beta \xi \sum_{q=1}^{2n} \xi_q \sum_{\ell' = 2\ell+1}^{2\ell} (-1)^{\ell'+1} e^{-2i \sum_{q=2\ell+1}^{2\ell' \ell+1} \xi_q} \]  

(E.48)

\[ \langle \downarrow \mid \prod_{q=1}^{2\ell} \left( e^{i\xi_q \sigma^z} e^{i(-1)^{q+1} \beta \sigma^x} \right) \sigma^+_i \prod_{q=2\ell+1}^{2n} \left( e^{i\xi_q \sigma^z} e^{i(-1)^{q+1} \beta \sigma^x} \right) \mid \downarrow \rangle \]  

(E.49)

\[ \approx \beta \xi \sum_{q=1}^{2n} \xi_q \sum_{\ell' = 1}^{2\ell} (-1)^{\ell'+1} e^{2i \sum_{q=2\ell+1}^{2\ell' \ell+1} \xi_q} \]  

(E.50)

\[ \langle \uparrow \mid \prod_{q=1}^{2\ell} \left( e^{i\xi_q \sigma^z} e^{i(-1)^{q+1} \beta \sigma^x} \right) \sigma^-_i \prod_{q=2\ell+1}^{2n} \left( e^{i\xi_q \sigma^z} e^{i(-1)^{q+1} \beta \sigma^x} \right) \mid \uparrow \rangle \]  

(E.51)

\[ \approx \beta \xi \sum_{q=1}^{2n} \xi_q \sum_{\ell' = 1}^{2\ell} (-1)^{\ell'+1} e^{-2i \sum_{q=2\ell+1}^{2\ell' \ell+1} \xi_q} \]  

Now we consider the different cases.
Only One of the Spins \(i\) and \(j\) Initially Up

Therefore considering the case where the spin \(i\) is initially up and the spin \(j\) is initially down, we have,

\[
\langle \prod_{q=1}^{2\ell} \left( e^{i\xi_q (\sigma_i^z + \sigma_j^z)} e^{i(-1)^{q+1}\beta (\sigma_i^x + \sigma_j^x)} \right) \sigma_i^+ \sigma_j^- \rangle 
\cdot \prod_{q=2\ell+1}^{2n} \left( e^{i\xi_q (\sigma_i^z + \sigma_j^z)} e^{i(-1)^{q+1}\beta (\sigma_i^x + \sigma_j^x)} \right) \rangle \tag{E.52}
\]

\[
\approx -\beta_i \beta_j \left[ 2n - 2\ell + 2 \sum_{\ell' = 2\ell + 2}^{2n} \sum_{\ell'' = 2\ell + 1}^{\ell' - 1} (-1)^{\ell' + \ell''} \cos \left( 2 \sum_{q=\ell''+1}^{\ell'} \xi_q \right) \right]
\]

\[
\langle \prod_{q=1}^{2\ell} \left( e^{i\xi_q (\sigma_i^z + \sigma_j^z)} e^{i(-1)^{q+1}\beta (\sigma_i^x + \sigma_j^x)} \right) \sigma_i^- \sigma_j^+ \rangle 
\cdot \prod_{q=2\ell+1}^{2n} \left( e^{i\xi_q (\sigma_i^z + \sigma_j^z)} e^{i(-1)^{q+1}\beta (\sigma_i^x + \sigma_j^x)} \right) \rangle \tag{E.53}
\]

\[
\approx -\beta_i \beta_j \left[ 2\ell + 2 \sum_{\ell' = 2}^{2\ell} \sum_{\ell'' = 1}^{\ell' - 1} (-1)^{\ell' + \ell''} \cos \left( 2 \sum_{q=\ell''+1}^{\ell'} \xi_q \right) \right]
\]
Thus

\[
\langle \uparrow \uparrow | \sigma_i^+ \sigma_j^- \rangle (t) \approx -\beta_i \beta_j \sum_{n=0}^{\infty} \left( \frac{-i\Delta_0 t}{2} \right)^{2n} \sum_{\ell=0}^{n} \frac{1}{(2\ell)! (2n-2\ell)!} \int \frac{d^{2n} \xi}{(2\pi)^{2n}}
\]

\[
\cdot \exp \left\{ -n\beta^2 (N-2) - (N-1)^2 \sum_{\ell'=1}^{2n-1} \sum_{\ell''=\ell'}^{2n} (-1)^{\ell''} \cos \left( 2 \sum_{q=\ell''+1}^{\ell'} \xi_q \right) \right\}
\]

\[
\approx -\beta_i \beta_j \sum_{n=0}^{\infty} \left( \frac{-i\Delta_0 t}{2} \right)^{2n} \sum_{\ell=0}^{n} \frac{1}{(2\ell)! (2n-2\ell)!} \int \frac{d^{2n} \chi}{(2\pi)^{2n}}
\]

\[
\cdot \exp \left\{ -n\beta^2 (N-2) - (N-1)^2 \sum_{\ell'=1}^{2n-1} \sum_{\ell''=\ell'}^{2n} \cos(\chi_{\ell'} - \chi_{\ell''}) \right\}
\]

\[
\approx -\beta_i \beta_j \sum_{n=0}^{\infty} \left( \frac{-i\Delta_0 t}{2} \right)^{2n} \sum_{\ell=0}^{n} \frac{1}{(2\ell)! (2n-2\ell)!} \int \frac{d^{2n} \chi}{(2\pi)^{2n}}
\]

\[
\cdot \exp \left\{ -n\beta^2 (N-2) - (N-1)^2 \sum_{\ell'=1}^{2n-1} \sum_{\ell''=\ell'}^{2n} \cos(\chi_{\ell'} - \chi_{\ell''}) \right\}
\]

\[
\approx -\beta_i \beta_j \sum_{n=0}^{\infty} \left( \frac{-i\Delta_0 t}{2} \right)^{2n} \sum_{\ell=0}^{n} \frac{1}{(2\ell)! (2n-2\ell)!} \int \frac{d^{2n} \chi}{(2\pi)^{2n}}
\]

\[
\cdot \exp \left\{ -n\beta^2 (N-2) - (N-1)^2 \sum_{\ell'=1}^{2n-1} \sum_{\ell''=\ell'}^{2n} \cos(\chi_{\ell'} - \chi_{\ell''}) \right\}
\]

\[
\cdot \left[ 2n - 2\ell + 2 \sum_{p=2\ell+2}^{2n-1} \sum_{q=2\ell+1}^{p-1} \cos(\chi_p - \chi_q) \right]
\]

\[
= -\beta_i \beta_j \sum_{n=0}^{\infty} \left( \frac{-i\Delta_0 t}{2} \right)^{2n} \sum_{\ell=0}^{n} \frac{1}{(2\ell)! (2n-2\ell)!} \int \frac{d^{2n} \chi}{(2\pi)^{2n}}
\]

\[
\cdot \exp \left\{ -n\beta^2 (N-2) - (N-1)^2 \sum_{\ell'=1}^{2n-1} \sum_{\ell''=\ell'}^{2n} \cos(\chi_{\ell'} - \chi_{\ell''}) \right\} \exp \left\{ -iX_1 (\cos \chi_1 + \cos \chi_2) - iX_2 (\sin \chi_1 + \sin \chi_2) \right\}
\]

In equation (E.55) we have introduced \( \chi \) variables just like in the appendix E.1. Then in equation (E.56) we use same steps leading equation (7.64), as well as making use of the fact that each of the terms over the sums over \( p \) and \( q \) in equation (E.55) are identical. The integral in equation (E.56) can be evaluated:

\[
\int \frac{d^2 \chi}{(2\pi)^2} \cos(\chi_1 - \chi_2) \exp \left\{ -iX_1 (\cos \chi_1 + \cos \chi_2) - iX_2 (\sin \chi_1 + \sin \chi_2) \right\}
\]

\[
= \int \frac{d^2 \chi}{(2\pi)^2} \cos(\chi_1 - \chi_2) e^{-iX_1 (\cos \chi_1 + \cos \chi_2)}
\]

\[
= \left( \int \frac{d\chi}{2\pi} \cos \chi_1 e^{-iX \cos \chi_1} \right)^2 + \left( \int \frac{d\chi}{2\pi} \sin \chi_1 e^{-iX \cos \chi_1} \right)^2
\]

\[
= - [J_1(X)]^2.
\]
Therefore we have

\[ \langle \uparrow \uparrow | \sigma_i^+ \sigma_j^- \rangle (t) \]

\[ \approx -\beta_i \beta_j \sum_{n=0}^{\infty} \left( \frac{-i\Delta_0 t}{2} \right)^{2n} \left[ \sum_{\ell=0}^{2n} \frac{2n - 2\ell}{(2\ell)!} \int dX P(X) [J_0(X)]^{2n} \right] \]

\[ + \sum_{\ell=0}^{n-1} \frac{(2n - 1 - 2\ell)(2n - 2\ell)}{(2\ell)!} \int \frac{dX}{(2\pi)} \frac{e^{-\frac{X^2}{2N\beta}}}{2N\beta} [J_0(X)]^{2n-2} \int \frac{d^2\chi}{(2\pi)^2} \cos(\chi_1 - \chi_2) \exp\{ -iX_1(\cos \chi_1 + \cos \chi_2) - iX_2(\sin \chi_1 + \sin \chi_2) \} \].

\[ \approx \frac{\beta_i \beta_j}{4} \int dX P(X) \left\{ [\Delta_0 J_0(X)t] \sin[\Delta_0 J_0(X)t] \right\} \]

\[ - \frac{1}{2} [\Delta_0 J_1(X)t]^2 (\cos[\Delta_0 J_0(X)t] + 1). \]
Similar calculations give:

\[
\langle | \uparrow \rangle \langle \uparrow | \sigma_i^- \sigma_j^+ \rangle (t) \\
\approx \frac{\beta_i \beta_j}{4} \int dX P(X) \left\{ [\Delta_0 J_0(X)t] \sin[\Delta_0 J_0(X)t] \\
- \frac{1}{2} [\Delta_0 J_1(X)t]^2 (\cos[\Delta_0 J_0(X)t] + 1) \right\} \tag{E.62}
\]

\[
\langle | \downarrow \rangle \langle \downarrow | \sigma_i^+ \sigma_j^- \rangle (t) \\
\approx -\frac{\beta_i \beta_j}{4} \int dX P(X) \left\{ [\Delta_0 J_0(X)t] \sin[\Delta_0 J_0(X)t] \\
- \frac{1}{2} [\Delta_0 J_1(X)t]^2 (\cos[\Delta_0 J_0(X)t] - 1) \right\} \tag{E.63}
\]

\[
\langle | \downarrow \rangle \langle \downarrow | \sigma_i^+ \sigma_j^+ \rangle (t) \\
\approx -i \frac{\beta_i \beta_j}{4} \int dX P(X) \left\{ [\Delta_0 J_0(X)t] (\cos[\Delta_0 J_0(X)t] - 1) \right. \\
\left. + \frac{1}{2} [\Delta_0 J_1(X)t]^2 \sin[\Delta_0 J_0(X)t] \right\} \tag{E.64}
\]

\[
\langle | \uparrow \rangle \langle \downarrow | \sigma_i^+ \sigma_j^- \rangle (t) \\
\approx -i \frac{\beta_i \beta_j}{4} \int dX P(X) \left\{ [\Delta_0 J_0(X)t] (\cos[\Delta_0 J_0(X)t] + 1) \right. \\
\left. + \frac{1}{2} [\Delta_0 J_1(X)t]^2 \sin[\Delta_0 J_0(X)t] \right\} \tag{E.65}
\]

\[
\langle | \uparrow \rangle \langle \downarrow | \sigma_i^- \sigma_j^- \rangle (t) \\
\approx -i \frac{\beta_i \beta_j}{4} \int dX P(X) \left\{ [\Delta_0 J_0(X)t] (\cos[\Delta_0 J_0(X)t] + 1) \right. \\
\left. + \frac{1}{2} [\Delta_0 J_1(X)t]^2 \sin[\Delta_0 J_0(X)t] \right\}. \tag{E.66}
\]
Combining the expressions (E.61-E.67) we get the following expressions for the desired correlators, at leading order in our approximations

\[ \langle \sigma^x_i \sigma^x_j \rangle = \langle \sigma^y_i \sigma^y_j \rangle = -\left( \Delta_0 t \right)^2 \int dX P(X) |J_1(X)|^2 \]  
(E.67)

\[ \langle \sigma^x_i \sigma^y_j \rangle = \langle \sigma^y_i \sigma^x_j \rangle = 0 \]  
(E.68)

\[ \langle \tau^x \sigma^x_i \sigma^x_j \rangle = \langle \tau^x \sigma^y_i \sigma^y_j \rangle = 0 \]  
(E.69)

\[ \langle \tau^x \sigma^x_i \sigma^y_j \rangle = -\langle \tau^x \sigma^y_i \sigma^x_j \rangle = \Delta_0 t \int dX P(X) J_0(X) \]  
(E.70)

\[ \langle \tau^y \sigma^x_i \sigma^x_j \rangle = \langle \tau^y \sigma^y_i \sigma^y_j \rangle = \beta_i \beta_j \int dX P(X) \left\{ [\Delta_0 J_0(X) t] \cos(\Delta_0 J_0(X) t) \right. \]  
\[ + \frac{1}{2} [\Delta_0 J_1(X) t]^2 \sin(\Delta_0 J_0(X) t) \right\} \]  
(E.71)

\[ \langle \tau^y \sigma^y_i \sigma^x_j \rangle = \langle \tau^x \sigma^y_i \sigma^y_j \rangle = 0 \]  
(E.72)

\[ \langle \tau^x \sigma^x_i \sigma^y_j \rangle = \langle \tau^y \sigma^y_i \sigma^x_j \rangle = \frac{\beta_i \beta_j}{2} \int dX P(X) \left\{ [\Delta_0 J_0(X) t] \sin(\Delta_0 J_0(X) t) \right. \]  
\[ - \frac{1}{2} [\Delta_0 J_1(X) t]^2 \cos(\Delta_0 J_0(X) t) \right\} \]  
(E.73)

\[ \langle \tau^y \sigma^y_i \sigma^y_j \rangle = \langle \tau^x \sigma^y_i \sigma^x_j \rangle = 0. \]  
(E.74)

When Both Spins \( i \) and \( j \) are Initially Up (or Down)

In this case similar steps to those in section E.3.1 lead to

\[ \left\langle \left| \uparrow \right\rangle \left\langle \left| \uparrow \right\rangle \left| \sigma^+_i \sigma^-_j \right. \right\rangle (t) \right. \]  
\[ = \beta_i \beta_j \sum_{n=2}^{\infty} \left( \frac{-i \Delta_0 t}{2} \right)^n \int dX P(X) [J_1(X)]^2 [J_0(X)]^{2n-2} \]  
(E.75)

\[ \cdot \sum_{\ell=1}^{n} \frac{(2n-2\ell)!(2\ell)!}{(2\ell)!}\frac{2n-2\ell)!}{2^{2n-3}} \]  
(E.76)

\[ = \beta_i \beta_j \frac{(\Delta_0 t)^2}{8} \int dX P(X) [J_1(X)]^2 [1 - \cos(\Delta_0 J_0(X) t)] \] .
Similarly

\[
\langle \downarrow \uparrow \downarrow \uparrow | \sigma_i^+ \sigma_j^- \rangle (t)
= \beta_i \beta_j \frac{(\Delta_0 t)^2}{8} \int dX P(X) [J_1(X)]^2 (1 + \cos(\Delta_0 J_0(X) t)) \quad (E.77)
\]

\[
\langle \downarrow \downarrow \uparrow \uparrow | \sigma_i^+ \sigma_j^- \rangle (t)
= i \beta_i \beta_j \frac{(\Delta_0 t)^2}{8} \int dX P(X) [J_1(X)]^2 \sin[\Delta_0 J_0(X) t] \quad (E.78)
\]

\[
\langle \downarrow \uparrow \downarrow \downarrow | \sigma_i^+ \sigma_j^- \rangle (t)
= -i \beta_i \beta_j \frac{(\Delta_0 t)^2}{8} \int dX P(X) [J_1(X)]^2 \sin[\Delta_0 J_0(X) t]. \quad (E.79)
\]

So we have

\[
\langle \tau^z \sigma^z_i \sigma^z_j \rangle = -\langle \tau^z \sigma^y_i \sigma^y_j \rangle \quad (E.80)
\]

\[
\langle \tau^x \sigma^x_i \sigma^x_j \rangle =\langle \tau^x \sigma^y_i \sigma^y_j \rangle = 0 \quad (E.81)
\]

\[
\langle \tau^x \sigma^x_i \sigma^y_j \rangle =\langle \tau^x \sigma^y_i \sigma^x_j \rangle =\langle \tau^y \sigma^x_i \sigma^y_j \rangle = 0 \quad (E.82)
\]

\[
\langle \tau^y \sigma^x_i \sigma^x_j \rangle =\langle \tau^y \sigma^y_i \sigma^y_j \rangle =\langle \tau^y \sigma^x_i \sigma^y_j \rangle = 0 \quad (E.83)
\]

\[
\langle \tau^y \sigma^x_i \sigma^x_j \rangle =\langle \tau^y \sigma^y_i \sigma^y_j \rangle = 0 \quad (E.84)
\]

E.3.2 Correlators Involving Longitudinal Components of the Bath Spins

We begin by computing the contribution to \( \langle \downarrow \uparrow \downarrow \uparrow | \sigma^z_i \rangle (t) \) from the initial central spin density matrix \( \hat{\rho}_S(0) = | \uparrow \rangle \langle \uparrow | \).

In the leading order orthogonality blocking approximation

\[
\langle \downarrow \uparrow \downarrow \uparrow | \sigma^z_i \rangle (t)
\approx \sum_{n=0}^{\infty} \left( \frac{-i \Delta_0}{2} \right)^{2n} \sum_{\ell=0}^{n} \int \{D\tilde{\eta}\}^{2\ell} \int \{D\eta\}^{2n-2\ell} \prod_{q=1}^{2\ell} \left( \Psi_0 U^{-1}(q+1) \right) (\sigma^z_i) \prod_{q=2\ell+1}^{2n} \left( \Psi_0 U^{-1}(q+1) \right) \right). \quad (E.85)
\]
Now
\[
\langle \eta_i | \prod_{q=1}^{2\ell} (e^{i\xi_q \sigma_z^i} e^{i(-1)^{q+1} \beta \sigma_z^i}) \sigma_z^i \prod_{q=2\ell+1}^{2n} (e^{i\xi_q \sigma_z^i} e^{i(-1)^{q+1} \beta \sigma_z^i}) | \eta_i \rangle \quad (E.86)
\]
\[
\approx \eta_i e^{in_0 \sum \xi_k} \exp \left\{ -n_0 \beta_i^2 - \beta_i^2 \sum_{p=1}^{2\ell-1} \sum_{q=p+1}^{2\ell} n(-1)^{p+q} e^{-2in_0 \sum_{k=p+1}^{\ell} \xi_k} + \beta_i^2 \sum_{p=1}^{2n-1} \sum_{q=p+1}^{2n} (-1)^{q+p} e^{-2in_0 \sum_{k=p+1}^{\ell} \xi_k} \right\}.
\]

Thus
\[
\langle \uparrow \uparrow | \sigma_z^i \rangle (t)
\]
\[
\approx \eta_i \sum_{n=0}^{\infty} \frac{(-i \Delta t)}{2} \sum_{\ell=0}^{n} \frac{1}{(2\ell)!} \frac{1}{(2n-2\ell)!} \int_0^{2\pi} \frac{d^{2n} \xi}{(2\pi)^{2n}} e^{-\delta K_i^{(n\ell)}(\xi_k)} \cdot \exp \left\{ -nN \beta^2 - N \beta^2 \sum_{\ell=1}^{2n-1} \sum_{\ell'=\ell+1}^{2n} (-1)^{\ell+\ell'} \cos \left( 2 \sum_{\ell=\ell'+1}^{\ell'} \xi_{\ell'} \right) \right\} \quad (E.87)
\]

where \( \delta K_i^{(n\ell)}(\xi_k) \) is a small change in the “action”,
\[
\delta K_i^{(n\ell)}(\xi_k) = \beta_i^2 \sum_{p=1}^{2n-1} \sum_{q=\ell}^{2n} (-1)^p q e^{-2in_0 \sum_{k=p+1}^{\ell} \xi_k}.
\] (E.88)

If, as we have been assuming in the rest of the text \( \beta_i \approx \beta \) and \( N \gg 1 \) then the change in the action is dominated by the rest of the “action” in equation \( E.87 \). In this case we recover the result stated in section \( E.3 \) (that is, in this case \( \langle \uparrow \uparrow \rangle (\sigma_z^i \rangle (t) \approx \eta_i \langle \uparrow \uparrow \rangle \rangle (t) \) . This argument is general to all correlators between central spin operators and \( \sigma_z^i \).

### E.3.3 Calculations of Correlators When There is a Small Bias on the Central Qubit

Here we show how the results described in section \( 8.1.1 \) were calculated. We calculate a set of correlators that are needed to calculate \( \langle \tau^x \sigma^x \sigma^x \rangle \) and \( \langle \tau^y \sigma^x \sigma^x \rangle \), in the precessional decoherence case, when there is a small additional bias \( \xi_0 \ll \omega_0 \). In this case the orthogonality blocking approximation is still valid, but the wave functions accumulate phase according to the bias on the central qubit. We calculated the
needed correlators for the cases where \( i \) and \( j \) are initially both spin up (or down) and when one is initially spin up. In all cases we have to deal with a phase factor of the form

\[
\left( \int_0^t dt_n \cdots \int_0^{t_2} dt_1 \int_0^t d\tilde{t}_n \cdots \int_0^{\tilde{t}_2} d\tilde{t}_1 \right) \cdot \exp \left\{ -i \sum_{\ell=0}^{n} (-1)^{\ell} (t_{\ell+1} - t_{\ell}) \xi_0 + i \sum_{\ell=0}^{n} (-1)^{\ell} (\tilde{t}_{\ell+1} - \tilde{t}_{\ell}) \xi_0 \right\},
\]

every term in the transition expansion. Here \( s_0 \) and \( \tilde{s}_0 \) specify the central qubit’s initial matrix element (in all cases we consider in this section \( s_0 = \tilde{s}_0 = 1 \)), and it is understood that we will set \( t_n = \tilde{t}_n = t \). Expressions like (E.89) can be taken care of by taking Laplace transforms with respect to \( t \) and \( \tilde{t} \), after inverting this transform one gets

\[
\left( \int_0^t dt_n \cdots \int_0^{t_2} dt_1 \int_0^t d\tilde{t}_n \cdots \int_0^{\tilde{t}_2} d\tilde{t}_1 \right) \cdot \exp \left\{ -i \sum_{\ell=0}^{n} (-1)^{\ell} (t_{\ell+1} - t_{\ell}) \xi_0 + i \sum_{\ell=0}^{n} (-1)^{\ell} (\tilde{t}_{\ell+1} - \tilde{t}_{\ell}) \xi_0 \right\},
\]

\[
\int_{-i\infty}^{i\infty} dz_1 \int_{-i\infty}^{i\infty} dz_2 e^{(z_1 + z_2) t} \prod_{\ell=0}^{n} \frac{1}{z_1 + i \xi_0 / 2} \prod_{\ell=0}^{n} \frac{1}{z_2 + i \xi_0 / 2}.
\]

**Only One of the Spins \( i \) and \( j \) is Initially Up**

We begin by computing the contribution to \( \langle \uparrow \uparrow \mid \sigma_i^+ \sigma_j^- \rangle(t) \) from the initial central spin density matrix \( \bar{\rho}_S(0) = \langle \uparrow \uparrow \rangle \). To leading order in the orthogonality blocking approximation, using the Laplace transform identity (E.90), we get

\[
\langle \uparrow \uparrow \mid \sigma_i^+ \sigma_j^- \rangle(t) \approx \int_{-i\infty}^{i\infty} d^2 z \frac{e^{(z_1 + z_2) t}}{(z_1 + i \xi_0 / 2)(z_2 - i \xi_0 / 2)} \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \left( \frac{-i \Delta_0}{2} \right)^{2(n+m)} \cdot \left( \frac{1}{z_1^2 + \xi_0^2 / 4} \right)^m \left( \frac{1}{z_2^2 + \xi_0^2 / 4} \right)^n \cdot \left\{ \prod_{q=1}^{2m} \left( \mathcal{P}_0 U(-1)^{q+1} \right) \right\} \left\{ \prod_{q=1}^{2n} \left( \mathcal{P}_0 U(-1)^{q+1} \right) \right\} \cdot \left( \sigma_i^+ \sigma_j^- \right)^2 \prod_{q=1}^{2n} \left( \mathcal{P}_0 U(-1)^{q+1} \right).
\]

(E.91)
Then using the usual maneuvers we have, the most secular terms in the transition expansion

\[
\langle \uparrow \downarrow \mid \uparrow \sigma_i^+ \sigma_j^- \rangle (t) 
\approx \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \left( \frac{-i\Delta_0}{2} \right)^{2(n+m)} \int_{-i\infty}^{i\infty} d^2z 
\cdot \left[ \frac{e^{(z_1+z_2)t}}{(z_1 + i\xi_0/2)(z_2 - i\xi_0/2)} \left( \frac{1}{z_1^2 + i\xi_0^2} \right)^{m} \left( \frac{1}{z_2^2 + i\xi_0^2} \right)^{n} \int \frac{d^2(n+m)\xi}{(2\pi)^2(n+m)} \right.
\cdot \exp \left\{ -(n + m)\beta^2(N - 2) - (N - 1)\beta^2 \sum_{\ell'=1}^{2(n+m)-1} \sum_{\ell''=\ell'}^{2(n+m)} (-1)^{\ell'+\ell''} \cos \left( 2 \sum_{q=\ell''+1}^{\ell'} \xi_q \right) \right\} 
\cdot \prod_{q=1}^{2(n+m)} \left( e^{i\xi_q(\sigma_i^+ + \sigma_j^+)} e^{i(-1)^{q+1}\beta(\sigma_i^+ + \sigma_j^+)} \right) \right).
\]

\[
(E.93)
\]

\[
\approx -\beta_i\beta_j \int_{-i\infty}^{i\infty} d^2z \cdot e^{(z_1+z_2)t} \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \left( \frac{-i\Delta_0}{2} \right)^{2(n+m)} 
\cdot \left[ \frac{1}{z_1^2 + i\xi_0^2} \right]^{m} \left[ \frac{1}{z_2^2 + i\xi_0^2} \right]^{n} \int \frac{d^2(n+m)\xi}{(2\pi)^2(n+m)} 
\cdot \exp \left\{ -(n + m)\beta^2(N - 2) - (N - 1)\beta^2 \sum_{\ell'=1}^{2(n+m)-1} \sum_{\ell''=\ell'}^{2(n+m)} (-1)^{\ell'+\ell''} \cos \left( 2 \sum_{q=\ell''+1}^{\ell'} \xi_q \right) \right\} 
\cdot \prod_{p=2m+1}^{2n+2} \sum_{p=2m+2}^{p-1} \sum_{k=q+1}^{p} (-1)^{p+q} \cos \left( 2 \sum_{k=q+1}^{p} \xi_k \right) 
\]

\[
(E.94)
\]

\[
\approx -\beta_i\beta_j \int_{-i\infty}^{i\infty} d^2z \cdot e^{(z_1+z_2)t} \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \left( \frac{-i\Delta_0}{2} \right)^{2(n+m)} 
\cdot \left[ \frac{1}{z_1^2 + i\xi_0^2} \right]^{m} \left[ \frac{1}{z_2^2 + i\xi_0^2} \right]^{n} \int \frac{d^2(n+m)\chi}{(2\pi)^2(n+m)} 
\cdot \exp \left\{ -(n + m)\beta^2(N - 2) - (N - 1)\beta^2 \sum_{\ell'=1}^{2(n+m)-1} \sum_{\ell''=\ell'}^{2(n+m)} \cos (\chi_{\ell'} - \chi_{\ell''}) \right\} 
\cdot \prod_{p=2m+1}^{2n+2} \sum_{p=2m+2}^{p-1} \sum_{q=2m+1}^{\ell'} \cos (\chi_p - \chi_q) 
\]

\[
(E.95)
\]

\[
= -\beta_i\beta_j \int dXP(X) \int_{-i\infty}^{i\infty} d^2z \cdot e^{(z_1+z_2)t} \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \left( \frac{-i\Delta_0}{2} \right)^{2(n+m)} 
\cdot \left[ J_0(X) \right]^{2(n+m)-1} \left[ 2n[J_0(X)]^2 - 2n(2n - 1)[J_1(X)]^2 \right] 
\]

\[
(E.96)
\]

\[
= -\beta_i\beta_j \int dXP(X) \int_{-i\infty}^{i\infty} d^2z \cdot e^{(z_1+z_2)t} \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \left( \frac{-i\Delta_0}{2} \right)^{2(n+m)} 
\cdot \left[ J_0(X) \right]^{2(n+m)-2} \left[ 2n[J_0(X)]^2 - 2n(2n - 1)[J_1(X)]^2 \right] 
\]

\[
(E.97)
\]

\[
= -\beta_i\beta_j \int dXP(X) \int_{-i\infty}^{i\infty} d^2z \cdot e^{(z_1+z_2)t} \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \left( \frac{-i\Delta_0}{2} \right)^{2(n+m)} 
\cdot \left[ J_0(X) \right]^{2(n+m)-2} \left[ 2n[J_0(X)]^2 - 2n(2n - 1)[J_1(X)]^2 \right] 
\]

\[
(E.98)
\]
So inverting the Laplace transformation (we have used Mathematica software for this),

\[
\langle \uparrow \uparrow | \sigma_i^+ \sigma_j^- \rangle (t)
\]

\[
= -\beta_i \beta_j \int dX \mathbb{P}(X) \frac{\Delta_0^2}{16 \Omega^6} \left[ \xi_0 \sin \left( \frac{t \Omega}{2} \right) + i \Omega \cos \left( \frac{t \Omega}{2} \right) \right]
\]

\[
\cdot \left\{ \sin \left( \frac{t \Omega}{2} \right) \left[ J_0(X)^2 \left( 3 \Delta_0^2 J_1(X)^2 \left( -12 \xi_0 + t \Omega^2 (\xi_0 t + 2i) \right) - 16 \xi_0 \Omega^2 + 8it\Omega^4 \right) \right.
\]

\[
+ J_1(X)^2 \left( 12 \xi_0^3 + t \Omega^4 (\xi_0 t - 6i) - \xi_0 \Omega^2 (-4 + \xi_0 t (\xi_0 t + 2i)) \right) \]

\[
+ t \Omega \cos \left( \frac{t \Omega}{2} \right) \left( J_0(X)^2 \left[ 8 \xi_0 \Omega^2 + 3 \Delta_0^2 J_1(X)^2 \left( 6 \xi_0 - it\Omega^2 \right) \right.ight.
\]

\[
- J_1(X)^2 \left( 6 \xi_0^3 + \xi_0 \Omega^2 (2 - i \xi_0 t) + it\Omega^4 \right) \}
\]

with

\[
\Omega = \Omega(X) \equiv \sqrt{[\Delta_0 J_0(X)]^2 + \xi_0^2}.
\]

Expressions such as (E.99) are difficult to understand and for our purposes will be used to generate values on a graph anyway. So for the remainder of this section we will give expressions for the other correlators we require in the form of a series like
\( (E.98) \), which can be resolved using Mathematica.

\[
\langle \psi | \psi | \sigma^+_i \sigma^-_j \rangle (t) \\
\approx \beta_i \beta_j \int dX P(X) \int_{-i\infty}^{i\infty} d^2 z e^{i(z_1 + z_2)t} \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \left( \frac{-i\Delta_0}{2} \right)^{2(n+m)+2} \\
\cdot \sum_{\ell=0}^{n} \left( \frac{1}{z_1^2 + \xi_0^2/4} \right)^{m+1} \left( \frac{1}{z_2^2 + \xi_0^2/4} \right)^{n+1} \\
\cdot [J_0(X)]^{2(n+m)} \left[ (2n+1)[J_0(X)]^2 - (2n+1)2n[J_1(X)]^2 \right] \\
(E.101)
\]

\[
\langle \psi | \psi | \sigma^+_i \sigma^-_j \rangle (t) \\
\approx -\beta_i \beta_j \int dX P(X) \int_{-i\infty}^{i\infty} d^2 z e^{i(z_1 + z_2)t} \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \left( \frac{-i\Delta_0}{2} \right)^{2(n+m)+1} \\
\cdot \left( \frac{1}{z_1^2 + \xi_0^2/4} \right)^{m+1} \left( \frac{1}{z_2^2 + \xi_0^2/4} \right)^{n} \\
\cdot [J_0(X)]^{2(n+m)-1} \left[ 2n[J_0(X)]^2 - 2n(2n-1)[J_1(X)]^2 \right] \\
(E.102)
\]

\[
\langle \uparrow \psi | \psi | \sigma^+_i \sigma^-_j \rangle (t) \\
\approx \beta_i \beta_j \int dX P(X) \int_{-i\infty}^{i\infty} d^2 z e^{i(z_1 + z_2)t} \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \left( \frac{-i\Delta_0}{2} \right)^{2(n+m)+1} \\
\cdot \left( \frac{1}{z_1^2 + \xi_0^2/4} \right)^{m} \left( \frac{1}{z_2^2 + \xi_0^2/4} \right)^{n+1} \\
\cdot [J_0(X)]^{2(n+m)-1} \left[ (2n+1)[J_0(X)]^2 - (2n+1)2n[J_1(X)]^2 \right]. \\
(E.103)
\]
Both \(i\) and \(j\) Initially Up (or Down)

Considering the case where both the spins \(i\) and \(j\) are initially up (or down), we have,

\[
\langle \uparrow \uparrow | \sigma^+_i \sigma^-_j \rangle (t) = \beta_i \beta_j \int dX P(X) \int_{-\infty}^{\infty} d^2 z e^{(z_1 + z_2)t} \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \left( \frac{-i \Delta_0}{2} \right)^{2(n+m+1)}
\]

(E.104)

\[
\cdot \left( \frac{1}{z_1^2 + \xi_0^2/4} \right)^{m+1} \left( \frac{1}{z_2^2 + \xi_0^2/4} \right)^{n+1}
\]

\[
\cdot [J_0(X)]^{2(n+m)-1}(2n+1)(2m+1)[J_1(X)]^2
\]

\[
\langle \downarrow \downarrow | \sigma^+_i \sigma^-_j \rangle (t) = -\beta_i \beta_j \int dX P(X) \int_{-\infty}^{\infty} d^2 z e^{(z_1 + z_2)t} \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \left( \frac{-i \Delta_0}{2} \right)^{2(n+m+1)}
\]

(E.105)

\[
\cdot \sum_{\ell=0}^{n} \left( \frac{1}{z_1^2 + \xi_0^2/4} \right)^{\ell+1} \left( \frac{1}{z_2^2 + \xi_0^2/4} \right)^{n+1}
\]

\[
\cdot [J_0(X)]^{2(n+m)-1}(2n+1)(2m+1)[J_1(X)]^2
\]

\[
\langle \uparrow \downarrow | \sigma^+_i \sigma^-_j \rangle (t) = \beta_i \beta_j \int dX P(X) \int_{-\infty}^{\infty} d^2 z e^{(z_1 + z_2)t} \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \left( \frac{-i \Delta_0}{2} \right)^{2(n+m+1)}
\]

(E.106)

\[
\cdot \left( \frac{1}{z_1^2 + \xi_0^2/4} \right)^{m+1} \left( \frac{1}{z_2^2 + \xi_0^2/4} \right)^{n+1}
\]

\[
\cdot [J_0(X)]^{2(n+m)-1}(2n+1)(2m+1)[J_1(X)]^2
\]

\[
\langle \downarrow \uparrow | \sigma^+_i \sigma^-_j \rangle (t) = -\beta_i \beta_j \int dX P(X) \int_{-\infty}^{\infty} d^2 z e^{(z_1 + z_2)t} \sum_{n=0}^{\infty} \sum_{m=0}^{\infty} \left( \frac{-i \Delta_0}{2} \right)^{2(n+m+1)}
\]

(E.107)

\[
\cdot \left( \frac{1}{z_1^2 + \xi_0^2/4} \right)^{m+1} \left( \frac{1}{z_2^2 + \xi_0^2/4} \right)^{n+1}
\]

\[
\cdot [J_0(X)]^{2(n+m)-1}(2n+1)(2m+1)[J_1(X)]^2
\]
Appendix F

Some Steepest Descents Integrals

F.1 Gaussian Average of a Green function

Consider the integral

\[ I_1 \equiv \frac{1}{2} \int_{-\infty}^{\infty} d\xi \frac{\xi^2}{\sqrt{2\pi}\sigma} e^{\frac{-\xi^2}{2\sigma^2}} \cos \left( t\sqrt{\Delta_0^2 + \xi^2} \right) \]  (F.1)

for \( \Delta_0 t \gg 1 \). Begin by substituting \( \omega = \sqrt{\xi^2 - \Delta_0^2} \)

\[ I_1 = \text{Re} \int_{\Delta_0}^{\infty} d\omega \frac{\omega}{\sqrt{\omega^2 - \Delta_0^2}} \frac{e^{-\frac{\omega^2 - \Delta_0^2}{2\sigma^2}} e^{i\omega t}}{\sqrt{2\pi}\sigma} \]  (F.2)

\[ = \frac{1}{\sqrt{2\pi}\sigma} \text{Re} e^{i\Delta_0 t} \int_{0}^{\infty} d\omega \frac{\omega + \Delta_0}{\sqrt{\omega(\omega + 2\Delta_0)}} \exp \left\{ \frac{-\omega^2}{2\sigma^2} + (it - \Delta_0\sigma^{-2})\omega \right\}. \]  (F.3)

In the last step we have made the substitution \( \omega \rightarrow \omega + \Delta_0 \). The above working gives the following useful formula which can be used to evaluate integrals of the form

\[ \int_{-\infty}^{\infty} \frac{d\xi}{\sqrt{2\pi}\sigma^2} e^{-\frac{\xi^2}{2\sigma^2} + i\xi^2 + \Delta_0^2 t} f(\xi) \]  (F.4)

\[ = \sqrt{\frac{2}{\pi}\sigma^2} e^{i\Delta_0 t} \int_{0}^{\infty} d\omega \left( \frac{\omega + \Delta_0}{\sqrt{\omega(\omega + 2\Delta_0)}} \right) G[f] \left( \sqrt{(\omega + \Delta_0)^2 - \Delta_0^2} \right) e^{-\frac{\omega^2}{2\sigma^2} + (it - \Delta_0\sigma^{-2})\omega} \]

where \( G[f](\xi) = \frac{1}{2} [f(\xi) + f(-\xi)] \) is the symmetrised version of the function \( f(\xi) \). As this is a Fourier one could obtain the long time behavior for \( I_1 \) by expanding \( \frac{\omega + \Delta_0}{\sqrt{\omega(\omega + 2\Delta_0)}} e^{-\frac{\omega^2}{2\sigma^2}} \) around \( \omega = 0 \) where the Fourier transform is not smooth [66] this would give use \( I_1 \sim \text{Re}Ce^{i\Delta_0 t}/\sigma\sqrt{t} \) which does not recover the behavior of the integral as \( \sigma \rightarrow 0 \) so a more sophisticated approach must be taken. To obtain an approximation to \( I_1 \) for \( t\Delta_0 \gg 1 \) which holds no matter how small \( \sigma \) we use the method of steepest decent. We deform the contour of integration in the complex plane so that the real part of the exponent \( -\frac{\omega^2}{2\sigma^2} + (it - \Delta_0\sigma^{-2})\omega \) decreases most
Figure F.1: The contour used in the steepest descents integral. The shaded colour shows the real part of the exponent in equation (F.3). The dashed line is deformed to the filled line along which the real part of the exponent decreases most rapidly. The contribution from the vertical line vanishes as it is moved to positive infinity along the real axis.

rapidly (see figure [F.1]). This will be along the curve where the imaginary part of the integral exponent is zero. Along this contour we may expand about the point at which the real part of the exponent is maximised this is the origin. Evaluating the gradient of the real part of the exponent:

$$-\nabla \text{Re} \left[ -\frac{(x+iy)^2}{2\sigma^2} + (it - \Delta_0 \sigma^{-2})(x+iy) \right]_{x=y=0} = \left( \frac{\Delta_0}{\sigma^2} r \right)$$

(F.5)

so that we should substitute $\omega = re^{i\vartheta}$ with $\tan \vartheta = \frac{t\sigma^2}{\Delta_0}$ and then expand about $\omega = 0$ which gives

$$\mathcal{J}_1 = \sqrt{\frac{\Delta_0}{\pi}} \text{Re} \left\{ \frac{e^{i\Delta_0 t + i\vartheta/2}}{2\sigma} \right\} \int_{0}^{\infty} \frac{dr}{\sqrt{r}} \exp \left( -\sqrt{\frac{t^2 \sigma^4 + \Delta_0^2}{\sigma^2}} r \right)$$

(F.6)

$$= \frac{1}{2} \left( \frac{t^2 \sigma^4}{\Delta_0^2} + 1 \right)^{-\frac{1}{2}} \cos \left( \Delta_0 t + \frac{1}{2} \vartheta \right)$$

(F.7)
F.2 Lorentzian Average

Consider the integral
\[ I_2 = \int_{-\infty}^{\infty} d\xi \frac{\gamma f(\xi)e^{i\sqrt{\xi^2 + \Delta_0^2}t}}{(\xi^2 + \gamma^2)} \]  \hspace{1cm} (F.8)

we are interested in a regime for which \( \Delta_0 t \gg 1 \) with no particular restriction on \( \gamma t \) but with \( \Delta_0 > \gamma \). \( f(\xi) \) is a function which is well behaved. The long time part of the Fourier transform can still be calculated by a steepest descent analysis, the point \( \xi = 0 \) is a saddle point for the exponent so integral will be dominated by the \( \xi = 0 \) the contribution from neighbourhood \( \xi = 0 \). In order to account for the fact that the poles of the lorentzian may be close too \( \xi = 0 \) we expand the prefactor to the exponential function
\[ \frac{\gamma f(\xi)e^{i\sqrt{\xi^2 + \Delta_0^2}t}}{(\xi^2 + \gamma^2)} = A_r(\xi) + A_+(\xi) + A_-(\xi) \]  \hspace{1cm} (F.9)

\[ A_+(\xi) = \frac{-if(i\gamma)}{2\pi(\xi - i\gamma)} \]  \hspace{1cm} (F.10)

\[ A_-(\xi) = \frac{if(-i\gamma)}{2\pi(\xi - i\gamma)} \]  \hspace{1cm} (F.11)

\[ A_r(\xi) = \frac{\gamma f(\xi)e^{i\sqrt{\xi^2 + \Delta_0^2}t}}{\pi (\xi^2 + \gamma^2)} - A_+(\xi) - A_-(\xi). \]  \hspace{1cm} (F.12)

Here we have split off the poles of the “amplitude function to leave a regularised part the integral \( I_2 \) can then be split up
\[ I_2 = I_{2+} + I_{2-} + I_{2r} \]  \hspace{1cm} (F.13)

\[ I_{2+} = \int_{-\infty}^{\infty} d\xi A_+(\xi)e^{i\sqrt{\xi^2 + \Delta_0^2}t} \]  \hspace{1cm} (F.14)

\[ I_{2-} = \int_{-\infty}^{\infty} d\xi A_-(\xi)e^{i\sqrt{\xi^2 + \Delta_0^2}t} \]  \hspace{1cm} (F.15)

\[ I_{2r} = \int_{-\infty}^{\infty} d\xi A_r(\xi)e^{i\sqrt{\xi^2 + \Delta_0^2}t}. \]  \hspace{1cm} (F.16)

Then expanding around the saddle point we find that along the steepest descent contour \( \xi \sim re^{i\frac{\pi}{2}} \) and that the exponent is \( i\Delta_0 t - \frac{r^2}{2\Delta_0} \) so that we find
\[ I_{2+} + I_{2-} \sim \frac{1}{2} \exp \left(-\frac{it\gamma^2}{2\Delta_0} + it\Delta_0\right) \left[ 1 + ifr \right] \left[ 1 + ierf \left( \frac{1 + ir}{2\sqrt{t_0}} \right) \right] \]  \hspace{1cm} (F.17)

\[ I_{2r} = e^{i\frac{\pi}{4}} \int_{-\infty}^{\infty} dr A_r\left(r e^{i\frac{\pi}{2}}\right) e^{i\Delta_0 t - \frac{r^2}{2\Delta_0}} \]  \hspace{1cm} (F.18)
where $A_r \left( re^{i\frac{\pi}{2}} \right)$ can be expanded around zero to give an approximation to $J_{2r}$. 