Quantum Decoherence and the Spin-Boson Model

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Abstract

In this report we provide a detailed introduction with regard to the fundamental concepts and notation of Quantum Entanglement and Quantum Decoherence. Having outlined the manner in which decoherence emerges as the result of considering the system of interest interacting with a (usually macroscopic) environment, we derive an approximate lower bound on the decoherence rate for the Scattering Model. Our derivation of the Scattering Model will demonstrate the necessity to introduce approximations in order that we may examine more complex situations. To this end in Ch.4 we develop the idea's of Master-Equations and Canonical Models which we combine in developing the Born-Markov Master-Equation for the Spin-Boson Model. Following this we solve precisely the Spin-Boson Model and justify the application of the so-called Non-Interacting Blip Approximation in the Ohmic case, noting that such a solution for the dynamics would allow reliable and accurate calculation of many quantities of practical interest such as the decoherence rate. The report is concluded with a summary and a brief introduction to the applications of decoherence in modern and possible future technologies.

Contents

Introduction

At the start of the 20th century clear holes were beginning to emerge in the framework of Newtonian Physics. Whereas relativity dealt with those objects on a huge scale such as galaxies and speeds approaching the speed of light, there were also incongruities between observed events and theoretical predictions on a microscopic level. This left many results unexplained by the standard theory and forced physicists to often proceed in an ad hoc fashion. One example of this which seems to have been the first explicit use of quantisation to solve these issues was Planck's solution to the problem of blackbody radiation. To solve this problem he modelled the constituent atoms of the material as harmonic oscillators and postulated that only a discrete set of frequencies could be obtained. While this yielded predictions which matched very accurately to those observed (given that exact blackbody radiation is not found in nature), it was as yet not founded on any solid theoretical footing and the quantisation was itself highly contentous since until this point, energy spectrums had been assumed continuous. The success of similar 'quantisation methods' in explaining observed phenomena such as the standard Zeeman effect, led to the laboured emergence of a new physics of the microscopic: 'quantum physics'. The mathematical basis for such a theory followed soon after in many different guises, with possibly the most famous being those of Heisenberg and Schrödinger, however throughout this process one question remained unanswered.

This problem with the new theory became known under the catch-all term of the 'measurement problem', which we will discuss at greater length in Ch.2. Here it will suffice to remark that whilst on a microscopic level, the theory and results demonstrated the existence of superpositions of states (an idea we will review in Ch.1), no such superpositions had ever been observed under macroscopic conditions. Further, when directly observed or 'measured' such superpositions 'collapsed' into a single classical state. The mechanism behind these observed results was not explained, it was simply held that a measurement on a superposition resulted in a classical state where the probabilities were determined by the state. This prompted several questions: firstly, how large is classical or small is microscopic? That is, at what point is something large enough that it is governed by classical laws? This was originally put in by hand and known as the Heisenberg cut, but this did not actually provide an answer, instead leaving a huge grey area. Second since any complete physical theory should be universally applicable, it follows that in some manner the classical laws are a macroscopic limit of the quantum laws, however the mechanism by which this occured was unknown.

It is these two questions which we shall concern ourselves with in the first few chapters, and it will emerge that the mechanism of "decoherence" resolves both problems by showing that there is no clean break but a gradation as classical physics emerge from the underlying quantum laws in the macroscopic case. We will then study this mechanism purely for its own sake, since it is a hugely interesting and potentially useful result. As can be seen even without the knowledge of what decoherence is or how it works. Let us consider that a full understanding of the mechanism by which classical physics emerge from quantum laws could, at least theoretically, allow us to slow or even halt the process. This would then allow us to create macroscopic superpositions (see Sect 1.1), or even allow us to perform multiple parallel computations simultaneously (see Ch.7). Indeed the possibility of employing macroscopic versions of quantum phenomena to manipulate and solve macroscopic 'problems' has become a huge area of research. It seems that a true appreciation of this topic and the possibilities offered by it, require a thorough understanding of decoherence.

This report is approximately divided into three regions. The first three chapters outline the phenomena which will be important to us and demonstrate the inability of classical physics to explain quantum results, before setting out the tools and notation to introduce and analyse decoherence. This culminates in the description and brief analysis of a simple model for decoherence where photons scatter off a macroscopic particle. The next three chapters consider ways of simplifying the process of obtaining results for more complex models through use of 'master-equations' and 'canonical models'. we then concentrate on the Spin-Boson model and obtain a master-equation for this model under certan assumptions (Ch.4) as well as exact equations (Ch.5) and in the case of 'ohmic dissipation' an approximation which we rigorously justify (Ch.6). For this case of ohmic dissipation we discuss the qualitative behaviour of the solution in different regions of phase-space and in one region gain qualitative estimates of the errors introduced by our approximation (see Appendix.A). We finally examine possible applications of our results in future technology. In particular we examine the role of decoherence in quantum computing and discuss ways in which it can be prevented from rendering our states classical by means of Quantum Error-Correcting Codes and Decoherence-Free Subspaces.

It would be impossible to fully capture such a wide and continually expanding field. However, I hope that I provided the reader with sufficient material so that they might appreciate the elgance and simplistic power of decoherence as a theory. I also hope that I have enthused the reader regarding the as yet unlocked potential of quantum technologies and the relvance of decoherence to these concepts.

1   Review of Quantum Phenomena

In this section we will review several of the major phenomena which result from quantum mechanics, looking in depth at the Superposition Principle, Quantum Tunneling and Quantum Entanglement. This will give us the key conceptual tools for our later introduction and analysis of decoherence. Each of these has been extensively studied and as such they are all well understood, thus this chapter in no way claims to be an exhaustive study of these results, but more of a primer. In each section some possible resources for further reading are indicated but there are many different sources and access to a moderate academic library should provide ample opportunity to study any topics in greater detail.

1.1   The Superposition Principle

At the heart of quantum mechanics is the principle of superposition, it is often the only result of quantum mechanics that people are aware of. Although it would be impossible to do a course in quantum mechanics without encountering the superposition principle, I will still briefly review it here due to the dependence of our later study of decoherence on a clear understanding of superposition. Indeed without superpositions there would be no need for terms like coherence and decoherence in quanum mechanics.

Quantum mechanical states are represented by vectors in the Hilbert Space. This is often the first lesson in quantum mechanics, despite the fact that it contains several abstract ideas and undefined terms, for example we shall not here go into the details of Hilbert Spaces except to say that they are complex vector spaces. Our initial statement also induces the question "What is an admissible state?" etc. but here we will not trouble ourselves with such subtleties. The superposition principle is now born from the linearity of the Hilbert Space.

Since quantum states are represented by vectors in a Hilbert Space we may form linear combinations of such vectors. If we envisage a Hilbert Space spanned by a set of orthonormal vectors labelled $|\psi_n\rangle$, then the superposition principle tells us that a linear combination of such vectors is an equally admissible state, e.g.

$$|\psi\rangle = \sum_n c_n |\psi_n\rangle \tag{1.1.1}$$

where $c_n \ \epsilon \ \mathbb{C}$ such that $\sum_n |c_n|^2 = 1$.

One well-known example of such superpositions are formed on a two-dimensional Hilbert Space (often measuring a "spin-half" particle). On this vector space our basis vectors are called $|0\rangle$ and $|1\rangle$ ("spin-up" and "spin-down") and we take an equally weighted linear combination of these vectors, meaning our new state is

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \tag{1.1.2}$$

and is such that $\langle\psi|\psi\rangle = 1$ (since the definition of orthonormal is $\langle i|j\rangle = \delta_{ij}$ and applies to our basis vectors $|0\rangle$ and $|1\rangle$), we therefore say that $|\psi\rangle$ is "normalized". We note that we can in fact take an uncountably infinite number of superpositions using just these two states $|\psi\rangle = p|0\rangle + q|1\rangle$ with $p, q\epsilon\mathbb{C}$ and $|p|^2 + |q|^2 = 1$, is then another acceptable normalized superposition.

The correct interpretation of superpositions has been a topic of hot contention since their discovery. The "standard" Copenhagen [1] interpretation of quantum mechanics regards the wavefunction $|\psi\rangle$ as a representation of something "real" that exists as more than a statistical description. Other interpretations regard the wavefunction $|\psi\rangle$ as merely a mathematical tool for calculating probabilities of measurements but not as such an element of the physical world, and thus not what Einstein would have called "an element of reality". I will not in this paper go into a detailed analysis and explanation of these different viewpoints. We will simply regard that in the sense that the wavefunction is a description of the behaviour of the system it "exists" and thus superpositions "exist".

The important division to be made here is between classical ensembles and quantum superpositions. In a classical ensemble (also called a proper mixture) the state $|\psi\rangle$ is in one of the states $|\psi_n\rangle$ but we do not know which one, we only know the probabilities of each one. In a superposition all states exist simultaneously and upon a measurement the probabilities for finding an eigenvalue is given by the modulus of the square of the coefficient of that eigenvector in the superposition. That is, if we have a superposition of non-degenerate eigenstates expressed as $\sum_n C_n|\psi_n\rangle$ our probability of measuring n is given by $|C_n|^2$. This can be easily generalized to the case of degenerate eigenstates. Therefore the superposition completely describes the probabilities of a measurement upon the system. Superficially our quantum situation seems analogous to our classical situation, however as we shall show below, this fails to explain quantum mechanical phenomena. In a quantum superposition, as mentioned earlier, each component is simultaneously present in the quantum state. This situation is referred to as a coherent superposition (but we shall usually just refer to it as a superposition), where coherence refers to the existence of simultaneously more than one classical quantity and a fixed phase between these quantities. Readers may be familiar with coherence as it applies to waves but we take an analogous definition for quantum states where coherence refers to a fixed relative phase between the components of a superposition. As such a coherent superposition is one in which all the states which sum together to create our overall state retain their relative phases.

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[1] The Copenhagen interpretation is so-called since it arose from the collaborative efforts of Niels Bohr and Werner Heisenberg whil they resided in Copenhagen around 1927. It was for many years the widely accpeted interpretation of qunatum mechanics but has recently fallen from favour since many physicists prefer interpretations such as Everetts many-worlds interpretation

The question we now ask is, "how can we experimentally demonstrate the existence of coherence and thereby show that a superposition is indeed different from an ensemble (i.e., a proper mixture) of its component states?" One way to do this is by an indirect confirmation of all components in the superposition by means of an interference experiment. I will briefly give an example of an interference experiment, but in a break from all tradition I will not consider the classic double-slit experiment, in spite of the remarks of Feynman that "[It] is absolutely impossible to explain in any classical way and has in it the heart of quantum mechanics. In reality, it contains the only mystery." from his 1963 lecture. Instead I will look at a slightly different experiment called a Mach-Zender Interferometer, as it not only nicely illustrates the superposition principle but also some other fascinating aspects of quantum mechanics

1.1.1 Mach-Zender Interferometer

A simple setup of the Mach-Zender Interferometer analogous to the double-slit experiment is shown above. In it a beam of light is emitted from a source and hits a half-silvered mirror, this has the effect of allowing half the photons through and reflecting the other half. These separate beams are then reflected off standard mirrors towards two detectors, which register a photon with a click. If we reduce the power of the source to emit a single photon (possibly through the selection of photons by successive polarizing sheets meaning only a very particular polarization is eventually transmitted). We would expect each experiment to result in one of the two detectors, A or B, to click depending on whether the photon was reflected or transmitted by the half silvered mirror
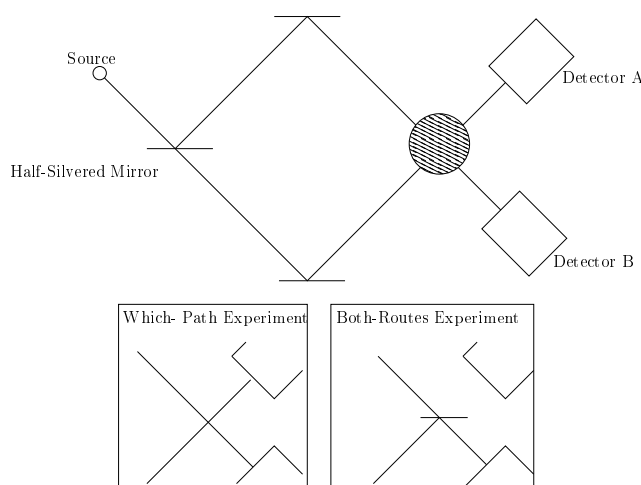

Figure 1: A Mach Zender Interferometer as described above, where the two different versions of the experiment are shown in the boxes.

Alternatively (as shown) we could place another half-silvered mirror at the point of intersection of the two reflected beams. The effect of this second half-silvered mirror is to create interference between the beams and result in only one of the two detectors registering photons. If we reduce the power of the source, so that single photons are omitted, then classically we would expect either detector to click approximately half of the time as a photon would be in only one of the two states '|transmitted⟩' or '|not transmitted⟩' but we do not know which and classically a photon cannot interfere with itself. However what is found is that only one detector ever clicks. Assuming the half-silvered mirror is a perfect 50-50 beam-splitter then the probability of the photon always being sent the same way for N independent experiments is $\frac{1}{2^N}$ and thus vanishingly small for many experiments. Therefore the only explanation is that the photon is in some sense both reflected and transmitted. Below we solve a slightly modified version of this experiment to explicitly demonstrate the effect of interference.

Let us imagine that the beam-splitter (in our example it was a half-silvered mirror but could also could be related to polarization etc.) transmits one "sort" of photon $|1\rangle$ and reflects another "sort" $|0\rangle$. Then if the initial state of the problem is $|0\rangle$ the beam-splitter sends it into $i|2\rangle + |3\rangle$ and similarly $|1\rangle \rightarrow |2\rangle + i|3\rangle$, the imaginary phase is a result of rotation by a right angle. Here state $|2\rangle$ represents the transmitted part of a state and $|3\rangle$ the reflected part. The primary property of a unitary transformation is that it sends orthogonal states into orthogonal states. So we verify

$$(-i\langle 2| + \langle 3|)(|2\rangle + i|3\rangle) = -i\langle 2|2\rangle + i\langle 3|3\rangle = i - i = 0 \tag{1.1.3}$$

and we conclude that they are indeed orthogonal.

The operator representing the beam-splitter is thus,

$$U_{BS1} = (i|2\rangle + |3\rangle)\langle 0| + (|2\rangle + i|3\rangle)\langle 1| \tag{1.1.4}$$

In the next stage of the interferometer $|2\rangle$ and $|3\rangle$ are both reflected via mirrors and thus pick up another imaginary phase due to reflection through a right-angle.

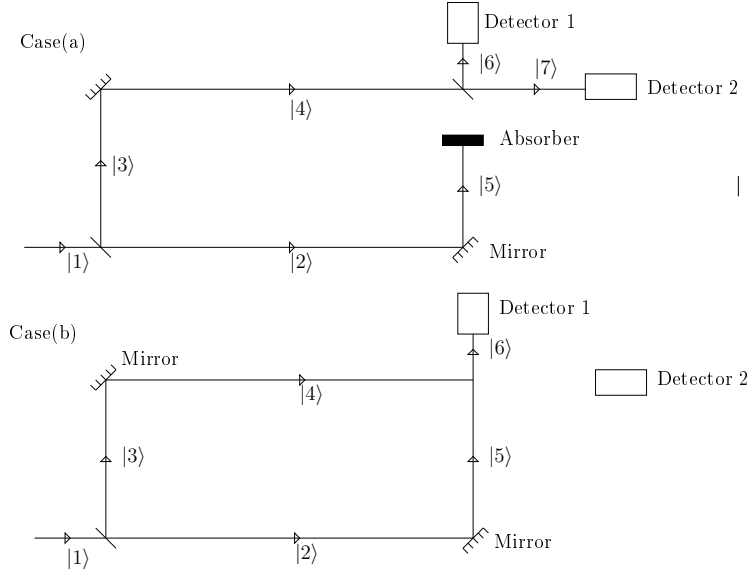$$U_{M1} = i|5\rangle\langle 2| \tag{1.1.5}$$

6

Figure 2: An alternative set-up of a Mach-Zender Interferometer, which is more conducive to our analysis. The two different forms of experiment are now distinguished by the inclusion or admission of an Absorber.

$$U_{M2} = i|4\rangle\langle 3| \tag{1.1.6}$$

Here clearly $|5\rangle$ represents the state $|2\rangle$ having been rotated by $90°$ and likewise $|4\rangle$ represents $|3\rangle$ after a $90°$ rotation. So after the mirrors, our states are transformed as,

$$|2\rangle + i|3\rangle \rightarrow i|5\rangle - |4\rangle \tag{1.1.7}$$

$$i|2\rangle + |3\rangle \rightarrow -|5\rangle + i|4\rangle \tag{1.1.8}$$

Finally the effect of the second beam splitter can be written as the operator

$$U_{BS2} = (i|6\rangle + |7\rangle)\langle 4| + (|6\rangle + i|7\rangle)\langle 5| \tag{1.1.9}$$

Here $|6\rangle$ is the state $|4\rangle$ having been reflected by our second beam-splitter or from the state $|5\rangle$ having been transmitted, the state $|7\rangle$ is the opposite of these (i.e. $|4\rangle$ transmitted or $|5\rangle$ reflected)

Let us imagine that we put an absorber in the path of the state $|5\rangle$ as shown in Fig.2. Thus the only state which reaches the second beam-splitter is $|4\rangle$ multiplied by an overall phase, thus after the second beam-splitter we are left with the eventual state $i|6\rangle + |7\rangle$ multiplied by an overall phase. This state corresponds to equal probabilities of measuring $|6\rangle$ and $|7\rangle$ corresponding ultimately to the two different detectors.

Without this absorber, and with the assumption that state $|1\rangle$ was sent, we find that after the first beam-splitter and the mirrors we are in the state $(i|5\rangle - |4\rangle)$ meaning the action of the second beam-splitter on this gives

$$\begin{aligned} U_{BS2}(i|5\rangle - |4\rangle) &= iU_{BS2}(|5\rangle) - U_{BS2}(|4\rangle) \\ &= i(i|6\rangle + |7\rangle) - (|6\rangle + i|7\rangle) \\ &= -2|6\rangle \end{aligned}$$

This is why as shown above the photons are only observed in detector 1.

Not only does this experiment nicely illustrate interference effects, it also poses several other questions. Wheeler asked: 'Can the experimenter choose whether the photon travels one direction or both' where such a question refers to our initial setup. If we return to our original Mach-Zender example, then we may envisage a situation where in the time between reflection by the conventional mirrors and intersection of the two beams we may choose whether or not to include the second half-silvered mirror. This is called a 'delayed-choice experiment' and allows us to choose after the event whether we want our photon to behave as a particle or a wave. That is, we can choose whether to perform a "which-route" or "both-routes" experiment. This is merely intended to show the problems with classical descriptions of quantum effects as in actuality the photon is not 'either' a particle or a wave, rather it is simultaneously both a particle and a wave, and through the action of decoherence the particle nature is obtained from the wavefunction. Indeed such experiments have been performed several times in the laboratory, but the most elegant example (in my opinion) is the one given by Wheeler of a quasar known as 0957+561A,B, which once thought to be two quasars, is now believed to be one. The light from this quasar is divided around an intervening galaxy which has the effect of a "gravitational lens". The galaxy takes two light rays spread apart

by approximately fifty-thousand light years on their way from the quasar and brings them back together again on Earth. We can perform a delayed-choice of experiment with the quasar acting as the half-silvered mirror and the intervening galaxy as the full mirrors in our setup. Thus by the inclusion or omission of a half-silvered mirror in our measuring apparatus we may perform our delayed-choice experiment, with photons separated by as much as fifty-thousand light years. This first experimental setup and subsequently this example are discussed very eloquently in the book Entanglement by Amir.D.Aczel, [7].

The final aspect of superposition I will mention here is regarding the scope of superpositions. The obvious question is that if we accept superposition as a principle, why is it that the classical world appears to us to constitute objects in a single place or in a single state of many other properties? If superpositions are a reality, why do I not have five copies of this page all swimming before my face in slightly different positions, in fact why stop at 5? This question boils down to the issue of measurement, indeed the measurement question has been a thorn in the side of quantum mechanics since the theory's invention. I hope later in this paper to convincingly illustrate the manner in which the classical world emerges from the governing quantum laws.

However, in the early days of the quantum theory to explain these incongruities between microscopic and macroscopic behaviour the 'cut-off' between the quantum and classical domains was usually put in arbitrarily by hand. The Heisenberg-cut in the standard Copenhagen Interpretation of quantum mechanics simply acted to ensure that microscopic objects were governed by quantum laws and macroscopic laws by classical physics. This was a most unsatisfactory explanation and since a boundary was never satisfactorily defined we can feel in many ways not a solution so much as a reformulation of the problem to pose as an answer. From this mess was born the theory of decoherence which will be the subject of much of the later paper.

In contrast to Heisenberg's cut, recent experiments have measured interference effects with increasingly large objects. To create an experiment of the strict double-slit variety for mesoscopic let alone macroscopic objects is very difficult since, although they have a de Broglie wavelength, it tends to be exceptionally small and the slits need to be of this order. Thus a slightly modified version of these interference experiments have to be set up to verify the wave nature of mesoscopic and macroscopic objects. An experiment based on the so-called Talbot-Lau effect (amongst others) has solved this problem. However it requires a large amount of advanced physics to understand this experiment and as such we will not go into it here. A brief explanation can be found in Sect 6.2 of [26] or the full experiment in either [18] or [19], where this second paper also focuses more on decoherence. It will suffice here to say that these experiments were done with C_{70} molecules which did indeed display the evidence expected for verification of the superposition principle and which fall into the mesoscopic range.

1.2 Tunneling in Quantum Mechanics

In Classical Mechanics, we envisage a situation where two regions in which a particle of any positive energy can reside, are divided by a barrier of potential energy with value V_0. Such a situation is shown in Fig.3 below. If we imagine a particle starts to the left of this bump, and has energy strictly less than V_0, classically this particle has 0 probability of ever being observed to the right of this potential barrier. This however is not the case in quantum mechanics as we shall demonstrate below.
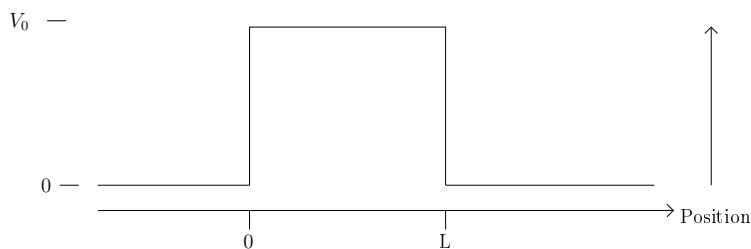
Figure 3: A diagrammatical representation of the one-dimensional potential we here consider.

We envisage a setting analogous to the one above with

$$V(x) = \begin{cases} 0 & \text{if } x < 0, \\ V_0 & \text{if } 0 < x < L, \\ 0 & \text{if } x > L. \end{cases} \tag{1.2.1}$$

So, since $\min V(x) = 0$ we know that only states with $E > 0$ can exist in this situation. Our asymptotic values are $V(-\infty)$ and $V(\infty) = 0$, So any state with $E > 0$ necesarrily oscillates as it goes to and from infinity. We now imagine our states have energy $0 < E < V_0$ and assume that particles are only transmitted from the left (i.e. $-\infty$), in order to simplify our problem.

Then for $x < 0$ we have the general state,

$$\psi_1(x) = A e^{\frac{ipx}{\hbar}} + B e^{\frac{-ipx}{\hbar}} \tag{1.2.2}$$

8

with $p = \sqrt{2mE} > 0$ and A, B ϵ $\mathbb{C}$. This is a general solution to the nonrelativistic standard Hamiltonian equation

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) + V(x)\psi(x) = E\psi(x) \tag{1.2.3}$$

with $E = \frac{p^2}{2m}$. Since at the point $x = 0$ we have a finite jump in potential, which enforces the conditions that $\psi(x)$ and $\frac{d}{dx}\psi(x) = \psi'(x)$ are both continuous at this point. This gives us two equations to satisfy,

$$\psi_1(0) = \psi_2(0)$$
$$\psi_1'(0) = \psi_2'(0) \tag{1.2.4}$$

If we write,

$$\psi_2(x) = C\sinh\frac{qx}{\hbar} + D\cosh\frac{qx}{\hbar} \tag{1.2.5}$$

with $q = \sqrt{2m(V_0 - E)} > 0$. Which again we could easily check is a general solution to the Hamiltonian equation in the Region 2. We then impose these conditions to get the two new relations:

$$A + B = D$$
$$ip(A - B) = qC \Rightarrow C = \frac{ip}{q}(A - B) \tag{1.2.6}$$

thus we can rewrite ψ_2 as,

$$\psi_2 = \frac{ip}{q}(A - B)\sinh\frac{qx}{\hbar} + (A + B)\cosh\frac{qx}{\hbar} \tag{1.2.7}$$

We now look at a general solution to the Hamiltonian in Region 3, but we also put the restriction that no particles are received from $+\infty$ (i.e. $p > 0$). This gives

$$\psi_3(x) = Ee^{\frac{ipx}{\hbar}} \tag{1.2.8}$$

Again a finite potential jump leaves us two conditions analogous to those in (1.2.4), namely

$$\psi_2(L) = \psi_3(L)$$
$$\psi_2'(L) = \psi_3'(L) \tag{1.2.9}$$

If we make the temporary substitution $sh \equiv \sinh\frac{qL}{\hbar}$ and $ch \equiv \cosh\frac{qL}{\hbar}$ then we can write these two relations in matrix format as,

$$\begin{bmatrix} \frac{ip}{q}\,\text{sh} + \text{ch} & -\frac{ip}{q}\,\text{sh} + \text{ch} \\ ip\,\text{ch} + q\,\text{sh} & -ip\,\text{ch} + q\,\text{sh} \end{bmatrix} \begin{bmatrix} A \\ B \end{bmatrix} = \begin{bmatrix} Ee^{\frac{ipL}{\hbar}} \\ ipEe^{\frac{ipL}{\hbar}} \end{bmatrix} \tag{1.2.10}$$

Now inverting the matrix we obtain expressions for A and B in terms of E. We will not go throught the details here, however the important result is that we obtain the expression for A,

$$A = -\frac{E}{2ip}e^{\frac{ipL}{\hbar}}\left(-2ip\,\text{ch} + \frac{q^2 - p^2}{q}\,\text{sh}\right) \tag{1.2.11}$$

We now note that size of E relates to the flow to $+\infty$ and A represents the rate of flow from $-\infty$. Thus we note that the constant $\frac{|E|^2}{|A|^2}$ measures the rate of transmission from $-\infty$ to $+\infty$ (a classically forbidden process). Thus we find,

$$T = \frac{|E|^2}{|A|^2} = \frac{4p^2}{\left[\frac{q^2-p^2}{q}\right]^2\sinh^2\frac{qL}{\hbar} + 4p^2\cosh^2\frac{qL}{\hbar}} = \frac{4p^2}{\left[\frac{q^2+p^2}{q}\right]^2\sinh^2\frac{qL}{\hbar} + 4p^2} \neq 0 \tag{1.2.12}$$

where the third equality comes from the relation $\cosh^2(x) - \sinh^2(x) = 1$. The important point here is that this transition coefficient is not zero, instead it depends on the energy of the particle and the step V_0 indirectly through p and q as well as the length L directly. Therefore our main result is that in quantum mechanics there is a non-zero probability that a particle may pass through a classically forbidden region into a different classically allowed region. This process is known as "Quantum Tunneling".

The history of quantum tunneling is a long and varied one. By 1928 George Gamov has solved the theory of the alpha decay of a nucleus via tunneling, before a seminar by George Gamov sparked Max Born into recognising the generality of quantum mechanical tunneling. His realization was that the scope of tunneling extended far past nuclear physics and is a general result of quantum mechanics that extends to many different systems. Quantum tunneling is used by enzymes to enhance reaction rates and is believed to play a role in the human sense of smell. Such examples are intended to demonstrate the wide application of the theory of quantum tunneling and hopefully illustrates how much tunneling has become an integral part of our understanding of the universe.

There is a huge amount of literature on quantum tunneling as is obvious from the range of applications mentioned in the previous paragraph, as such it would be impossible to try and summarize it here. However, as in the previous section it is interesting to note those experiments being done in the macroscopic domain, as this demonstrates the application of quantum laws to traditionally classical situations. An example of such experiments can be found in the paper [13] or alternately[27]. Since quantum tunneling will be implicitly used in our later work but a detailed physical understanding will be unnecessary, as such we choose not to analyze it further here.

1.3 Quantum Entanglement and Bell's Theorem

We shall now turn our attention to the phenomenon known as "Quantum Entanglement" which is the key process underlying our later work on decoherence. Entanglement, among others, was one of the properties which caused Einstein such discomfort with accepting the quantum theory as complete. Indeed it was Einstein who in 1935 along with Podolosky and Rosen formulated a paper in which they introduced the thought experiment that became known as the EPR paradox (although it should be stressed that this is not a paradox merely a curious result). He believed that this result demonstrated the incompleteness of the quantum picture and derided the results as "spukhafte fernwirrkung" which is usually translated as "spooky action at a distance". However quantum mechanics has prevailed with the effects and the strong correlations predicted by the theory being observed in numerous settings.

So, to elaborate on this last paragraph let us define entanglement, in this next section we will closely parallel parts of Section 2.3 of [26]. Let us envisage a state vector $|\psi\rangle$ on the Hilbert Space S, which is composed of two subsystems S_1 and S_2 (in this situation S would be called a bipartite quantum state). We call the state vector $|\psi\rangle$ entangled with respect to S_1 and S_2 if it cannot be decomposed into the tensor product of two states each residing in one of our two subsystems. That is, there does not exist $|\psi\rangle_1 \, \epsilon S_1$ and $|\phi\rangle_2 \, \epsilon S_2$ such that $|\psi\rangle = |\psi\rangle_1 \otimes |\phi\rangle_2$. Note that in the remainder of this paper we shall often omit the tensor-product symbol "$\otimes$" when expressing tensor-products of quantum states, (i.e. in the remainder of this paper $|\psi\rangle = |\psi\rangle_1 \otimes |\phi\rangle_2 = |\psi\rangle_1|\phi\rangle_2$). We shall however endeavour to retain the symbol whenever we refer to products of operators acting on different Hilbert Spaces or when we refer to the Hilbert Spaces themselves.

As an example of some entangled states, consider two spin-$\frac{1}{2}$ particles described by the mutually orthogonal basis states $|0\rangle_i$ and $|1\rangle_i$, $i = 1, 2$ of their respective two-dimensional Hilbert Spaces. From now on note that $|0\rangle \equiv$ 'up' and $|1\rangle \equiv$ 'down'. There are many different quantum states for the composite system which comprises two spin-$\frac{1}{2}$ particles being maximally entangled. Maximally entangled means that having made a measurement on the entangled basis of one subsystem, there is a change in the knowledge of the observer from a mixture of probabilities to a certainty that the state in the unmeasured Hilbert Space is in a eigenstate with known eigenvalue. Thus, any subsequent measurement on this second subsystem will yield one result with certainty and this result is known beforehand given the result of the measurement on the first subsystem. We will restrict our attention here to the states which are commonly referred to as Bell states and are given by

$$|\phi^{\pm}\rangle = \frac{1}{\sqrt{2}} \left(|0\rangle_1|0\rangle_2 \pm |1\rangle_1|1\rangle_2 \right)$$

$$|\psi^{\pm}\rangle = \frac{1}{\sqrt{2}} \left(|0\rangle_1|1\rangle_2 \pm |1\rangle_1|0\rangle_2 \right) \tag{1.3.1}$$

It is easy to explicitly show that these states cannot be expressed as a tensor product of states in the subsystem S_1 and S_2. For example if we take $|\phi^+\rangle$ then we would want to decompose it into two states

$$|\psi\rangle_1 \epsilon S_1 = a|0\rangle_1 + b|1\rangle_1$$

$$|\phi\rangle_2 \epsilon S_2 = c|0\rangle_2 + d|1\rangle_2 \tag{1.3.2}$$

where $a, b, c, d \, \epsilon \, \mathbb{C}$ as such these are the most general states allowed. Thus our composite state looks like:

$$|\psi\rangle_1|\phi\rangle_2 = ac|0\rangle_1|0\rangle_2 + ad|0\rangle_1|1\rangle_2 + bc|1\rangle_1|0\rangle_2 + bd|1\rangle_1|1\rangle_2 \tag{1.3.3}$$

which gives us the four equations $ac = \frac{1}{\sqrt{2}}$, $bc = 0$, $ad = 0$ and $bd = \frac{1}{\sqrt{2}}$. The second of these implies that either $b = 0$ or $c = 0$, then since $ac = \frac{1}{\sqrt{2}}$ we know $c \neq 0$ and similarly $bd = \frac{1}{\sqrt{2}}$ means $b \neq 0$. Therefore we have a contradiction and as claimed we cannot decompose $|\phi^+\rangle$ into a tensor product of two other states.

Let us look more closely at one of these states to really understand the concepts on which the EPR "paradox" was built, although we do not follow the exact format of the original problem, this more modern thought experiment captures the essential "oddness" of quantum entanglement. lets us suppose we have two spin-$\frac{1}{2}$ particles which at some time interact in such a way that their total spin, in for example the z-direction, is 0. Since they are spin-$\frac{1}{2}$ particles they must have spin either $+$ or $-$ corresponding to spin-up and spin-down. Once we know the spin of one particle then we can immediately infer the other particle has the opposite spin (this situation arises often in nature when two electrons are emitted with equal and opposite spins for example). Considering this case we can see it is the same as our state $|\psi_-\rangle$, where,

$$|\psi^{\pm}\rangle = |0\rangle_1|1\rangle_2 \pm |1\rangle_1|0\rangle_2$$

The point now is that our earlier work on superposition demonstrated that this is not analogous to a statistical treatment of the states where the states are equal and opposite in some direction but we are simply unaware of in which way. This means that both spin-$\frac{1}{2}$ states are simultaneously in spin-up and spin-down. Let us now make a measurement on state 1, which as we know acts as a projection operator onto the eigenstates of the operator. Thus after we have performed a measurement and normalized let us assume we measured spin-up we are left with the state (minus an arbitrary overall phase),

$$|0\rangle_1|1\rangle_2 \tag{1.3.4}$$

Which means the superposition has collapsed into the state where particle 1 is in the spin-up state and as such the superposition for particle 2 has also collapsed to the state where particle 2 is in the spin-down state. We notice that these particles are

no longer entangled and are indeed already in a separated state in our above equation. However the point of interest is that no measurement has been performed on state 2, indeed this whole process makes no reference to the position of particle 2 except that at some time it was local to particle 1 in order to create the entangled state. Thus if we regard the wavefunction as "real" then the collapse of the wavefunction and the transfer of information could have occurred faster than relativity permits. The important point here is that by making a measurement on the wavefunction we destroy it (i.e., collapse it into a set of degenerate eigenvectors). As we could show no full information has been transferred here, only partial information and thus relativity is not violated, this follows from the No-Cloning theorem which will be briefly demonstrated at the end of this paper however it is also indicated in many books such as [28].

If we were able to separate $|\psi\rangle$ into a tensor product of $|\psi\rangle_1$ and $|\phi\rangle_2$ then we know that these states are not entangled and we may regard these two systems as individual entities. By this we mean that each system possesses its own state vector which constitutes a complete description of the subsystem. This is equivalent to saying that any value which could be obtained from a measurement on the composite system could also be found to be equivalent by a measurement on the subsystems separately. Hence, although we can consider the quantum state as part of a larger composite system, the component states still retain their individuality (like the classical situation). On the other hand, if there exists no subsystem states $|\psi\rangle_1$ and $|\phi\rangle_2$ and as such $|\psi\rangle$ is entangled then this separability criterion has failed and we are no longer able to describe the state $|\psi\rangle_1$ in the Hilbert Space S_1 without reference to S_2. Thus entanglement, in some sense, removes the individuality of a particle, "measurement on part of the system is to be regarded as measurement on the whole system" (J.J.Sakurai Modern Quantum Mechanics [16]).

The peculiar features of entanglement have been confirmed by numerous experiments including on macroscopic scales, where photon pairs have been separated by distances of many kilometres. (For proof-of-principle experiments on entanglement see [24]) Entanglement is one of the corner stones of the "second quantum revolution" (see [17]) which refers to quantum technologies such as quantum computers and quantum cryptography. We will look at these in slightly more detail at the end of this paper, especially the role of decoherence in quantum computing.

1.3.1 Bell's Inequality and Theorem

We will here consider the state $|\psi^-\rangle$ more and attempt to demonstrate the level to which entanglement makes us abandon classical certainties and specifically "there can be no local hidden-variable theory consistent with quantum mechanics". Here 'local' is tricky to define, we mean to convey that locality upholds the tenet of special relativity that information cannot be transferred faster than the speed of light. This then requires a rigorous definition of 'information' which is a non-trivial and contentious task. Intuitively we say that 'locality' has been preserved if within our theory there is no mechanism by which an event can have an effect on another event outside of it's light-cone, this will be satisfactory for our purposes. This section is close throughout to Sect 3.9 in [16]

So, let us imagine that we have a pair of spin-$\frac{1}{2}$ particles described by the composite state,

$$|\psi\rangle = \frac{1}{\sqrt{2}} \left(|\hat{z}_+\rangle_1 |\hat{z}_+\rangle_2 - |\hat{z}_-\rangle_1 |\hat{z}_-\rangle_2 \right) \tag{1.3.5}$$

To simplify this notation slightly we will express $|\hat{z}_+\rangle_1 |\hat{z}_-\rangle_2$ as $|\hat{z}_+; \hat{z}_-\rangle$ where the first term in this state vector relates to particle 1 and thus $\mathbb{H}_1$ and the second to the second particle and $\mathbb{H}_2$. Thus our state can be rewritten:

$$|\psi\rangle = \frac{1}{\sqrt{2}} \left(|\hat{z}_+; \hat{z}_-\rangle - |\hat{z}_-; \hat{z}_+\rangle \right) \tag{1.3.6}$$

where we have explicitly indicated the quantisation direction. As we discussed before a measurement on this system would produce a 50-50 split between the two states $|\hat{z}_+; \hat{z}_-\rangle$ and $|\hat{z}_-; \hat{z}_+\rangle$ which correspond to particle 1 spin-up, particle 2 spin-down in the first case and the opposite for the second.

To be more pictorial, we envision this scenario as our two spin-$\frac{1}{2}$ particles moving in opposite directions towards two observers A and B who receive particle 1 and 2 respectively. If we imagine that observer A chooses to measure spin in the z-direction let us assume he finds it to be spin-up, then even before observer B has measured his particle, observer A knows the spin of the second particle. On the other hand, if A were not to measure his particle at all then B has an equal chance of getting spin-up or spin-down. At first glance this might not be very surprising, if we picture a situation where a particle with 0 charge collapses into two particles of opposite charge which move away from the point of collapse in opposite directions then we have an analogous situation where neither observer knows before a measurement which charge they will measure (positive or negative) but once they have measured their own particle they can infer the charge of the other particle. The quantum case is much more subtle than that since observers may choose to measure other observables instead of $\hat{S}_z$, for example $\hat{S}_x$.

Recall that for a spin-$\frac{1}{2}$ system the $\hat{S}_x$ eigenkets and the $\hat{S}_z$ eigenkets are related by the formulae:

$$|\hat{x}_\pm\rangle = \frac{1}{\sqrt{2}} \left(|\hat{z}_+\rangle \pm |\hat{z}_-\rangle \right)$$

$$|\hat{z}_\pm\rangle = \frac{1}{\sqrt{2}} \left(|\hat{x}_+\rangle \pm |\hat{x}_-\rangle \right) \tag{1.3.7}$$

11

Returning to our composite system this second pair of equations allows us to rewrite our original spin-singlet with the direction of quantization being the x-direction, which gives us:

$$|\psi\rangle = \frac{1}{\sqrt{2}} \left(|\hat{x}_+ ; \hat{x}_- \rangle - |\hat{x}_- ; \hat{x}_+ \rangle \right) \qquad (1.3.8)$$

Apart from the phase we could have guessed this intuitively from our original equation since spin-singlets have no preferred directions and we picked $\hat{z}$ arbitrarily. Suppose now that, rather than measuring $\hat{z}$, observer A decides to measure the spin of his particle in the $\hat{x}$ basis. Once observer A has measured his particle which without loss of generality we shall assume was spin-up in the x-direction then particle 2 will have collapsed into the eigenstate corresponding to spin-down in the x-direction, which we know from our earlier equation is equal to $\frac{1}{\sqrt{2}} \left(|\hat{z}_+\rangle - |\hat{z}_-\rangle \right)$ and observer B still has an equal chance of obtaining either result when they perform their measurement on the z-direction.

We note from this and the table below that the result of B's measurement depend on which axis A decides to measure in. Remember once again that A and B can be theoretically arbitrarily far apart, with no possibility of communications or mutual interactions. The orthodox quantum-mechanical interpretation of this state of affairs is that the measurement behaves like a selection process such that when observer A measures a basis, it is that basis and those states which observer A recorded that are 'selected'. The table below shows all possible results when observer A and observer B are both free to choose their direction of measurement.

Spin component for A	A's result	Spin component for B	B's result	Probability
z	+	z	-	0.5
z	-	z	+	0.5
z	+	x	+	0.25
z	+	x	-	0.25
z	-	x	+	0.25
z	-	x	-	0.25
x	+	x	-	0.5
x	-	x	+	0.5
x	+	z	+	0.25
x	+	z	-	0.25
x	-	z	+	0.25
x	-	z	-	0.25

This table illustrates clearly the way in which a selection of a basis by observer A alters the measurement statistics of observer B

Some physicists have argued that the conceptual sacrifices this requires us to make are inherent in the probabilistic nature of quantum mechanics and this probabilistic nature is a result of our incomplete information. That is, there are some so-called "hidden variables" which describe the behaviour of quantum systems in a deterministic fashion but we are as yet unaware of, or we are possibly unable to obtain information on these variables. That would mean in our example that prior to measurement all the characteristics of spin in our particles were decided, however we require our measurement obtain this information. This was most attractive as a theory since it negated the need for our instantaneous non-local collapse of the wavefunction. It was thought for a long time that it would be possible to set up a local hidden-variable description which fitted exactly with the results of the classical interpretation and as such these two interpretations would be equivalent. However in 1964 an Irish mathematician called John Stewart Bell described a method by which a local hidden-variable theory could be experimentally separated from the results of quantum mechanics as described by wavefunction collapse.

Note that here we do not follow Bell's original argument but that of E.P.Wigner which still retains all the essential features of the original. Although we know that for any particle it is impossible to simultaneously measure $\hat{S}_z$ and $\hat{S}_x$, however when we have a large number of spin-$\frac{1}{2}$ particles , we may assign a certain fraction of them to have the following property:

1. If $\hat{S}_z$ is measured we obtain a plus sign with certainty.
2. If $\hat{S}_x$ is measured we obtain a minus sign with certainty.

A particle which satisfies this property is therefore said to be of type $(\hat{z}_+ ; \hat{x}_-)$. Notice that we are not claiming that such measurements can be realised simultaneously we are instead asserting definite values for spins in more than one direction in the knowledge that only one component of the two can be measured. Let us now examine in what sense this model can account for the results of spin-correlation measurements made on a composite spin-singlet system. It should be obvious from our earlier discussions that there must be a perfect opposite matching between particle 1 and 2: if particle 1 is of type $(\hat{z}_+ ; \hat{x}_-)$ then particle 2 must be of the form $(\hat{z}_- ; \hat{x}_+)$. Thus we reproduce the correlation measurements if the particles are matched as

Particle 1		Particle 2	
$(\hat{z}_+ ; \hat{x}_-)$	$\leftrightarrow$	$(\hat{z}_- ; \hat{x}_+)$	α
$(\hat{z}_+ ; \hat{x}_+)$	$\leftrightarrow$	$(\hat{z}_- ; \hat{x}_-)$	β
$(\hat{z}_- ; \hat{x}_+)$	$\leftrightarrow$	$(\hat{z}_+ ; \hat{x}_-)$	γ
$(\hat{z}_- ; \hat{x}_-)$	$\leftrightarrow$	$(\hat{z}_+ ; \hat{x}_+)$	η

$(1.3.9)$

with equal populations throughout, meaning $\frac{1}{4}$ each. There is a subtle but key assumption implied here: suppose that a particle pair belongs tp type α and observer A decides to measure $\hat{S}_z$ of particle 1, then she clearly receives a plus sign regardless of whether B chooses to observe $\hat{S}_z$ or $\hat{S}_x$ of particle 2. It is in this sense that we are able to retain locality (this term is specifically defined as Einstein's locality principle, and effectively states that measurements performed on particle 1 do not instantaneously effect particle 2). In this model A's result is independent of B's choice of basis.

Thus far the two interpretations have been equivalent, however we now turn our attention to more-complicated situations where the model described above leads to different predictions from those of the usual quantum mechanical interpretations. We begin with three unit vectors $\bar{a}$, $\bar{b}$ and $\bar{c}$ which are in general not mutually orthogonal.
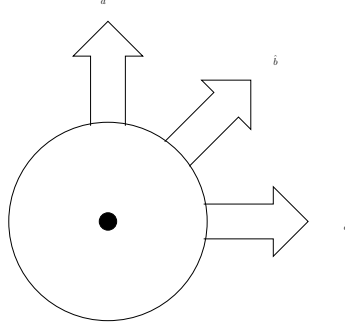

Figure 4: An example of three 'usable' direction vectors in a two-dimensional plane, labeled $\bar{a}$, $\bar{b}$ and $\bar{c}$

We follow an analogous "argument" to that applied above and assign each type $(\hat{a}, \hat{b}, \hat{c})$ a definite direction. So for example we would say that in the state $(\hat{a}_-, \hat{b}_-, \hat{c}_+)$ then a measurement of $\hat{S}_a$ would definitely result in a minus sign etc. (we once again stress that this model does not claim all three could be simultaneously known only that a proportion of states have this property where only one spin can ever be measured). We also retain the perfect opposite matching so that if particle 1 was measured as above, then particle 2 would necessarily be in the state $(\hat{a}_+, \hat{b}_+, \hat{c}_-)$. The table below shows the eight mutually exclusive possibilities the population of each is indicated in the first column.

Population of state	Particle 1	Particle 2
N_1	$(\hat{a}_+, \hat{b}_+, \hat{c}_+)$	$(\hat{a}_-, \hat{b}_-, \hat{c}_-)$
N_2	$(\hat{a}_+, \hat{b}_+, \hat{c}_-)$	$(\hat{a}_-, \hat{b}_-, \hat{c}_+)$
N_3	$(\hat{a}_+, \hat{b}_-, \hat{c}_+)$	$(\hat{a}_-, \hat{b}_+, \hat{c}_-)$
N_4	$(\hat{a}_+, \hat{b}_-, \hat{c}_-)$	$(\hat{a}_-, \hat{b}_+, \hat{c}_+)$
N_5	$(\hat{a}_-, \hat{b}_+, \hat{c}_+)$	$(\hat{a}_+, \hat{b}_-, \hat{c}_-)$
N_6	$(\hat{a}_-, \hat{b}_+, \hat{c}_-)$	$(\hat{a}_+, \hat{b}_-, \hat{c}_+)$
N_7	$(\hat{a}_-, \hat{b}_-, \hat{c}_+)$	$(\hat{a}_+, \hat{b}_+, \hat{c}_-)$
N_8	$(\hat{a}_-, \hat{b}_-, \hat{c}_-)$	$(\hat{a}_+, \hat{b}_+, \hat{c}_+)$

$$(1.3.10)$$

let us envisage a case where observer A finds $\hat{S}_a$ to be plus and observer B finds $\hat{S}_b$ to negative. It is clear from our table that the pair belong to type 1 or 2 (analogous cases can be made for the other values). So the number of particles for which this is realised is $N_1 + N_2$, and because the N_i are positive semi-definite we obtain relations such as

$$N_1 + N_2 \leq (N_1 + N_3) + (N_2 + N_6) \tag{1.3.11}$$

If we now define $P(\hat{a}_+; \hat{b}_-)$ to be the probability that in a random selection observer A measures $\hat{S}_a$ to be + and observer B measures $\hat{S}_b$ to be -. Then clearly from our table

$$P(\hat{a}_+; \hat{b}_-) = \frac{N_1 + N_2}{\sum_1^8 N_i} \tag{1.3.12}$$

We use this technique to also obtain

$$P(\hat{a}_+; \hat{c}_-) = \frac{N_1 + N_3}{\sum_1^8 N_i}$$

$$P(\hat{c}_-; \hat{b}_-) = \frac{N_2 + N_6}{\sum_1^8 N_i} \tag{1.3.13}$$

from these relations we derive that we can rewrite our inequality from earlier as:

$$P(\hat{a}_+; \hat{b}_-) \leq P(\hat{a}_+; \hat{c}_-) + P(\hat{c}_-; \hat{b}_-) \tag{1.3.14}$$

13

This is known as Bell's Inequality and it follows from Einstein's locality principle.

We now return to the world of quantum mechanics. In the classical interpretation we don't talk about a particular fraction of particle pairs, say $\frac{N_1}{\sum_1^8 N_i}$, belonging to type 1. Instead, we characterize all states by the same ket. With this state vector and the laws of quantum mechanics we are able to calculate each of the terms in Bell's inequality. Considering $P(\hat{a}_+; \hat{b}_-)$ firstly, it is clear that if observer B were directly opposite A then because of the exact opposite correlations previously discussed this observer would measure '-' with certainty. However if we consider a new quantization axis $\bar{b}$ that makes an angle θ_{ab} with $\bar{a}$. Once particle is measured as +, particle b falls into the eigenstate expressed in the $\hat{b}$ basis,

$$|\psi\rangle_2 = \cos\frac{\theta_{ab}}{2}|+\rangle - e^{i\phi} \sin\frac{\theta_{ab}}{2}|-\rangle \tag{1.3.15}$$

Where ϕ is an arbitrary phase which has no relevance to the probabilities. This therefore implies that the probability of measuring $\hat{b}$ to be spin-down is $\sin^2\frac{\theta_{ab}}{2}$. Thus we find

$$P(\hat{a}_+; \hat{b}_-) = \frac{1}{2} \sin^2\frac{\theta_{ab}}{2} \tag{1.3.16}$$

Where the factor $\frac{1}{2}$ arises from the probability of initially obtaining a plus with our measurement of $\hat{a}$. using this and a generalization of θ to the other terms, we can write Bell's Inequality as,

$$\sin^2\frac{\theta_{ab}}{2} \leq \sin^2\frac{\theta_{ac}}{2} + \sin^2\frac{\theta_{cb}}{2} \tag{1.3.17}$$

To show this is not always possible consider the case $\theta_{ab} = \frac{\pi}{2}$ and $\theta_{ac} = \theta_{cb} = \frac{\pi}{4}$ which would imply $1 \leq \frac{2}{\sqrt{2}} = \sqrt{2}$, which would be a contradiction. Therefore the quantum mechanical predictions relating to local hidden-variables are not equivalent to the classic interpretation. Indeed all interpretations based on Einstein's locality principle are thus experimentally different from those of the Copenhagen ilk.
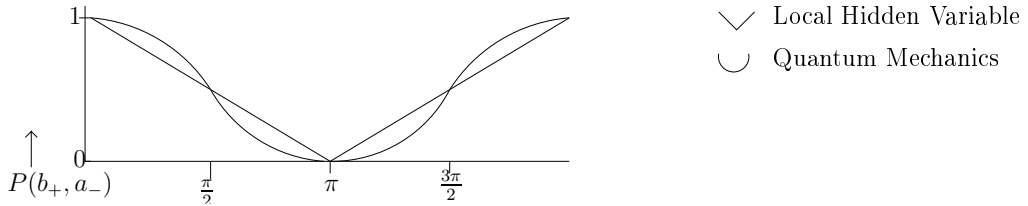

Figure 5: A comparison of results expected for our two different cases, local hidden variables and quantum mechanics, showing how for non-orthogonal angles the two models do not agree.

The findings of all recent precision experiments have conclusively established that Bell's inequality was violated, in one case by more than 9 standard deviations. What is more, in these experiments the results violate the inequalities in such a way as to (within error limits) fulfill the predictions of quantum mechanics. This should hopefully convince the reader that, in this issue, quantum mechanics has prevailed by a landslide. Thus any hidden-variable theorems must be non-local to satisfy experimental data and it seems most physicists are more willing to accept the wavefunction as "real" rather than abandon locality.

1.4 Summary

- In quantum mechanics we have superpositions constituting a linear combination of possible measurement results. Such a superposition, when expressed as an orthonormal basis and normalized, gives us the probabilities of a result of a measurement on the state, as the square of the coefficients of the degenerate eigenvectors.

- We showed that a quantum superposition has effects that cannot be explained by dismissing the superposition as a statistical description analogous to a classical ensemble. This was illustrated by the fact that in some sense all the components of the superposition simultaneously exist and can interact.

- We investigated a Mach-Zender Interferometer setup to demonstrate these effects such as constructive/destructive interference, and to mention some other interesting results from these experiments.

- We showed explicitly with a one-dimensional potential problem that in quantum mechanics a particle can travel between two classically allowed regions, even when they are divided by a barrier of potential energy greater than the energy of the particle. this phenomenon is called quantum tunneling.

- We defined entanglement and explicitly used Bell-states to demonstrate the non-classical correlations resulting from entanglement.

- We considered the implications for entanglement with (among others) regards to locality and discussed the key differences between quantum and classical correlations.

- We explicitly derived Bell's Inequality and also Bell's Theorem so that we could demonstrate that any 'hidden-variable' theory would have to be non-local and as such we firmly showed that classical physics is incapable of describing quantum phenomena.

2   Introduction to Decoherence

In this chapter, we will initially consider the "standard" formalism of quantum mechanics in terms of operators, bras and kets. We will not extensively review this formalism since almost all introductions to quantum mechanics begin with this method, those readers unfamiliar with it are recommended to consult any one of a multitude of introductory textbooks and briefly familiarise themselves with the basics. We are going to start by considering the shortfalls in this method and to what extent it can be considered 'complete'. Having identified the issues with the standard formalism we introduce some tools which we will later use to create our own subtly different system. These tools will primarily consist of 'density matrices' and their generalisation 'reduced density matrices', as well as the Von-Neumann measurement scheme which will be the mechanism which takes us from considering a quantum system interacting with a classical measurement apparatus to considering a situation where both components are described by the laws of quantum mechanics. Having developed our tools and given an introduction to our new scheme we will finally introduce decoherence and discuss its relevance to the aforementioned problems, discussing the ways our known result of quantum mechanics match with those of the new system. Hopefully after this chapter the reader will understand the fundamentals of a new system, accept its consistency with previous known results and appreciate its value in tackling some of the shortcomings of the operator formalism.

2.1   Problems with The Operator Formalism

The primary gap in the operator formalism is typically referred to as the "measurement problem", this name was chosen and is retained for purely historical reasons and is, as a result, slightly misleading. Firstly, the measurement problem is not a single problem, rather it is a collection of related problems and secondly, the problem extends beyond merely measurement in a classical sense. The measurement problem spans much of quantum mechanics, having roles in a multitude of aspects ranging from the interpretation of quantum mechanics to the distinctions which separate the macroscopic and microscopic domains. The measurement problem can be essentially captured in the more all-encompassing question regarding the quantum-to-classical transition i.e. "how does classical physics emerge from the underlying quantum laws?" We now break this into four sections, namely:

- The Problem of Outcomes - Why do measurements have outcomes at all? This aspect in particular of the measurement problem relies heavily on the readers own personal preference with regards to interpretation. Without more evidence (which may not even exist) such as an answer to the question: "Is it possible to construct a universe capable of sustaining life in which this were not the case?" It would not serve our purpose to debate the relative merits of different (currently) mutually compatible theories and as such I won't refer to this again.

- The Problem of Wavefunction Collapse - Again this issue relies heavily on the readers interpretation regarding the role of the wavefunction in quantum mechanics and whether it can be said to be an 'element of reality'. Decoherence certainly deals with the mechanism by which a superposition becomes a single pure state and thus if one regards the wavefunction as representing something 'real' then decoherence solves this problem.

- The Problem of Non-Interference - Why on macroscopic scales (and even mesoscopic scales) do we rarely observe interference effects. This question finds an elegant answer in the phenomenon of decoherence, and in the next couple of chapters this should become clear.

- The Problem of Preferred Basis - This ties in closely with our last problem. A solution to our previous point would explain why we do not experience mesoscopic superpositions, however the issue still arises that, depending on the scale of the system, the physically preferred quantities change. By this we mean that in the macroscopic limit we see objects in a single position whereas on the microscopic scale this is not necessarily the case even though both are interacting with the same environment. In the microscopic domain, a closed system (i.e., one not interacting with any external environment) 'selects' the energy eigenstates as the basis within which no superposition exists. Thus our question becomes: "what selects these bases?" Decoherence explains how the preferred basis is a result of the form of the interaction and as such does not have to be put in 'by hand'.

A full understanding of these problems is essential to the reader in order that they may appreciate the necessity and role of decoherence. When we consider these problems in terms of the operator formalism of quantum mechanics we understand why new tools are needed. The laws of this system state that when a measurement is made on a superposition in a certain basis, then the wavefunction collapses to a single eigenstate.

$$|\psi\rangle = \sum_i c_i |\psi_i\rangle \longrightarrow |\psi_i\rangle \tag{2.1.1}$$

Here the whole issue of how a state is selected is encapsulated within the arrow. The fact that a single eigenstate is selected is quite simply built into the system and as such the mechanism and reasons behind this cannot be investigated using this notation as it stands. This motivates the introduction of our tools and the Von-Neumann measurement scheme in order that we may break down this action into a form that we can analyze. Finally I will briefly note that these are the issues we must bear in mind as we develop our new system. In some ways the new formalism is more ambiguous and open to misinterpretation, however it is by these above criteria that we must judge it and with these issues in mind. This chapter is similar in content and aim to Ch.2 of [26] which introduces in the same notation these and other tools and is an excellent source for any reader who wishes to consider the material covered in this chapter in greater depth.

2.2 The Concept of Density Matrices

In this section we develop the concept of density matrices, beginning with so-called pure-state density matrices before looking at the generalizations of reduced density matrices and mixed state density matrices which require careful distinguishing from one another. The motivation behind our introduction of density matrices is that entanglement prevents us from assigning a simple state vector to describe our system, density matrices are our way of circumventing this problem. It will ultimately turn out that reduced density matrices provide an elegant way of describing the measurement statistics of a measurement on the system having taken any entanglement with another system into account, but not having to explicitly write in its influence.

2.2.1 Pure-State Density Matrices

We begin with a pure state described by the ket $|\psi\rangle$ and from this we then define the 'density operator' $\hat{\rho}$ as,

$$\hat{\rho} \equiv |\psi\rangle\langle\psi| \tag{2.2.1}$$

which we note is independent of any basis and acts as a projection operator onto $|\psi\rangle$. We shall often from here on use the term 'density matrix' interchangeably with density operator, however at this point we should make the distinction that a density matrix is a density operator expressed with respect to a particular basis $\{|\psi_i\rangle\}$. Despite this subtle distinction the term density matrix is widely used in the literature and as such having noted this we move on. However we will as much as possible denote the density operator by $\hat{\rho}$ and the density matrix by ρ.

If we now express our original state vector $|\psi\rangle$ as a superposition with respect to some complete orthonormal basis $\{|\psi_i\rangle\}$ as $\sum_i c_i|\psi_i\rangle$ then it follows that the density matrix becomes

$$\sum_{i,j} c_i c_j^* |\psi_i\rangle\langle\psi_j| \tag{2.2.2}$$

The terms in which $i \neq j$ are known as the interference terms and are the terms which embody the quantum coherence. Where by "coherence" we mean the existence of fixed phases between the different components which constitute our state vector $|\psi\rangle$. However it is important to note that these interference terms must be understood as existing with respect to our chosen basis. If we choose a basis such that there are no interference terms this is not equivalent to a classical situation since the basis may not be one that is familiar to us in a classical sense and a change of basis may restore interference terms. To illustrate this, consider a system which is constrained to two possible positions labelled $|0\rangle$ and $|1\rangle$, (such a situation is commonly referred to as a two-state system) and the superposition $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ which, as discussed in the first chapter, cannot be classically explained. In this case our density matrix in the basis $\{|0\rangle, |1\rangle\}$ would have $\frac{1}{2}$ in every position, that is a matrix given by

$$\begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix} \tag{2.2.3}$$

whereas if we change basis to $\left\{\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle), \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)\right\}$, then we could see that the superposition would now be written in this new basis as $|0'\rangle$ which would leave us with a density matrix given as

$$\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} \tag{2.2.4}$$

Which neatly illustrates our point that a diagonal density matrix does NOT necessarily correspond to a classical situation.

We now introduce the trace operation which is denoted as "Tr" and acts on some operator (e.g., our density operator $\hat{\rho}$) as follows. We choose an arbitrary orthonormal basis $\{|\phi_i\rangle\}$ for the Hilbert space of our system and perform the operation:

$$\text{Tr}(\hat{\rho}) = \sum_i \langle\phi_i|\hat{\rho}|\phi_i\rangle \tag{2.2.5}$$

which in matrix notation corresponds to taking the trace in the conventional sense. The important fact about the trace operation is that it is independent of the basis that is chosen. This result follows from standard linear algebra and a proof can be found in many books on the subject. The trace also has several useful properties that we shall use later such as

$$\text{Tr}(\hat{A}\hat{B}\hat{C}) = \text{Tr}(\hat{C}\hat{A}\hat{B}) = \text{Tr}(\hat{B}\hat{C}\hat{A}) \tag{2.2.6}$$

i.e. it is invariant under cyclic permutation. It is also a linear map which implies that

$$\text{Tr}(x\hat{A} + y\hat{B}) = x\text{Tr}(\hat{A}) + y\text{Tr}(\hat{B}) \tag{2.2.7}$$

With $x, y \epsilon \mathbb{R}$ scalars. Again these results can be proved using standard linear algebra, however for some semblance of brevity we shall not prove them here.

So, the question naturally arise as to why we introduce the trace function? To answer this we consider some hermitian operator $\hat{O}$ which represents some observable acting on our system described by our density operator $\hat{\rho}$. Then taking the

trace operation on the product of these and choosing to express the result in the basis of eigenvalues of the observable $\hat{O}$ which we denote $|o_i\rangle$ each with eigenvalues o_i (here we assume a discrete spectrum however the generalization is reasonably simple), then we obtain,

$$\text{Tr}(\hat{\rho}\hat{O}) = \sum_i o_i |\langle o_i|\psi\rangle|^2 \equiv \langle\hat{O}\rangle \tag{2.2.8}$$

where $\langle\hat{O}\rangle$ denotes the expected value of the observable $\hat{O}$ when it acts on the state vector $|\psi\rangle$. One immediate result from this is that if we set $\hat{O}$ to $\hat{I}$ (the identity operator), then $\text{Tr}(\hat{\rho}) = \langle\hat{I}\rangle = 1$. This is a result of the normalization of our state i.e. that $|\langle\psi|\psi\rangle|^2 = 1$. If we again inspect our equation for the trace operation we notice that, using the identity operator it is equivalent to the sum of the probabilities of possible measurements on our state. That is, the probability of measuring o_i on our state $|\psi\rangle$ is given by the overlap $|\langle o_i|\psi\rangle|^2$. This clearly illustrates why when using the identity operator, the sum over i must be equal to 1. Now consider $\text{Tr}(\hat{\rho}^2)$ which will because of the normalization of $|\psi\rangle$ still yield 1, i.e.

$$\text{Tr}(\hat{\rho}^2) = \sum_i \langle o_i|\psi\rangle\langle\psi|\psi\rangle\langle\psi|\o_i\rangle \tag{2.2.9}$$

$$= \sum_i \langle o_i|\psi\rangle\langle\psi|o_i\rangle \tag{2.2.10}$$

$$= \sum_i |\langle o_i|\psi\rangle|^2 = \sum o_i^2 = 1 \tag{2.2.11}$$

This fact that both $\text{Tr}(\hat{\rho})$ and $\text{Tr}(\hat{\rho}^2)$ equal one will become important later as a quick method of distinguishing pure-state density matrices from other 'types' of density matrices. We now continue to consider these other types of matrix.

2.2.2 Mixed State Density Matrices versus Reduced Density Matrices

So far density matrices have not yielded any improvement over the standard use of bra's and ket's in describing pure states. However, let us consider mixed states where there is, in addition to the possible existence of quantum superpositions, also a classical ignorance about the state. By way of example, consider a system which we know is in one of two states but definitely not in a superposition of the two states and there is an equal chance that it is one of the two states. We would not in the notation of bra's and ket's normally concern ourselves with this system since it is a classical problem not a quantum one, but we see that if we take an ensemble view, then we can still extract the measurement statistics on the system by expressing our state as,

$$|\psi\rangle = \frac{1}{2}|0\rangle + \frac{1}{2}|1\rangle \tag{2.2.12}$$

This corresponds to an ensemble situation where half the time the state is in the state $|0\rangle$ and the other half it's in $|1\rangle$. This is as discussed at great length not equivalent to a superposition since the sum of the squares of the coefficients does not equal one, i.e. that this state (assuming our states are orthonormal) is not normalized. We consider a more complicated case where we have a mixture of superpositions in classical ensemble, taking a pair of superpositions of our two orthonormal states $|0\rangle$ and $|1\rangle$, e.g. $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ and $\frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)$. Then if we imagine that each of these superpositions exist which probability half we get the mixed state,

$$\frac{1}{2}\left[\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) + \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)\right] \neq \frac{1}{\sqrt{2}}|0\rangle \tag{2.2.13}$$

Therefore, if we interpreted this as a superposition then we would be left with only the state $|0\rangle$ not correctly normalized. This does not make sense since we know that we have a classical ensemble of two superpositions and in each superposition the probabilities of measuring 0 and 1 are equal thus half the time a measurement will result in the state $|1\rangle$ which is in direct contradiction to the superposition interpretation. Such ensembles may arise in nature when a process creates a state with certain known probabilities but where the state itself for each occasion is not know. For example our first ensemble $\frac{1}{2}(|0\rangle + |1\rangle)$ could arise when a measurement is made on the superposition $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$, in the basis $\{|0\rangle, |1\rangle\}$.

If we use our density matrix and trace operations on these mixed states then we can still investigate expectation values and other values on our system. Now we express our set of possible states as $|\psi_i\rangle$ which have probability p_i in our ensemble. Then our density matrix will be of the form

$$\hat{\rho} = \sum_i p_i |\psi_i\rangle\langle\psi_i| \tag{2.2.14}$$

As such we calculate expectation values in the same way as before namely for a hermitian operator $\hat{O}$ which has a complete orthonormal basis $\{|o_j\rangle\}$, we calculate the expected value $\langle\hat{O}\rangle$ as $\text{Tr}(\hat{\rho}\hat{O})$, which is

$$\langle\hat{O}\rangle = \sum_i p_i \langle\psi_i|\hat{O}|\psi_i\rangle$$

$$= \sum_{i,j} p_i \cdot o_j \langle\psi_i|o_j\rangle \tag{2.2.15}$$

note here that $|\psi_i\rangle$ are not necessarily orthogonal. If we set our operator $\hat{O}$ above equal to the identity operator and as such evaluate $\text{Tr}(\hat{\rho})$ then we establish,

$$\text{Tr}(\hat{\rho}) = \sum_i p_i \langle \psi_i | \psi_i \rangle = \sum_i p_i \tag{2.2.16}$$

since these p_i are probabilities this must be equal to unity. Thus, as with the case of pure-state density matrices we find that $Tr(\hat{\rho}) = 1$. However, if we consider $\hat{\rho}^2$ we note a difference between the mixed-state density matrices and the pure-state density matrices. We see that,

$$\hat{\rho}^2 = \sum_{i,j} p_i p_j |\psi_i\rangle\langle\psi_i|\psi_j\rangle\langle\psi_j| \tag{2.2.17}$$

note that usually $\langle\psi_i|\psi_j\rangle \neq 0$, however even when the $\{|\psi_i\rangle\}$ is an orthonormal basis we would still have,

$$\hat{\rho}^2 = \sum_i p_i^2 |\psi_i\rangle\langle\psi_i| \tag{2.2.18}$$

which by taking the trace over we find $Tr(\hat{\rho}^2) = \sum_i p_i^2$ and this is strictly less than unity except in the case where $p_0 = 1$ which corresponds to the pure-state density matrix. At the risk of overstating the point it is important to specify when dealing with a mixed-state rather than a superposition because of the similarity of notation and the possibility that not all states will be constantly normalized, many people find it simpler to ignore normalization coefficients while working only to resurrect them at the end of a calculation which may lead to considerable confusion if not carefully distinguished. This is one strength of the density matrix approach; it automatically gives you a method for distinguishing mixed-states from pure superpositions.

Let us now change tack slightly and return to considering entangled states. Picture two systems denoted A and B which are entangled and in a pure-state, but where the observer only has access to one of these, without loss of generality let us say A. The question may well be asked: "What is the correct quantum mechanical object that encapsulates all possible measurement statistics for observables on A?". The answer turns out to be a reduced density matrix as we shall now demonstrate.

Let us consider a state vector which acts on our system comprising A and B in the form $|\psi\rangle = \sum_i^2 \frac{1}{\sqrt{2}}(|a_i\rangle|b_i\rangle)$ where $|a_i\rangle$ and $|b_i\rangle$ are the eigenstates of $\hat{A}$ and $\hat{B}$ respectively. The density matrix is therefore clearly,

$$\sum_{i,j}^2 \frac{1}{2}(|a_i\rangle\langle a_j| \otimes |b_i\rangle\langle b_j|) \tag{2.2.19}$$

What we eventually want to achieve is a matrix which although having the effect of the system B considered, makes reference only to system A as the system on which we can take measurements. To this end we take the "partial trace" over the system B which can be interpreted as averaging over the effects of B. We do this by taking the trace in the normal way but only with respect to the orthonormal basis $\{|\phi_l\rangle\}$ of B and not with respect to the orthonormal basis $\{|\psi_k\rangle\}$ of A. Denoting the partial trace over B by Tr_B we find,

$$\text{Tr}_B(\hat{\rho}) = \hat{\rho}_A = \frac{1}{2}\sum_l\sum_{i,j}|a_i\rangle\langle a_j|\langle\phi_l|b_i\rangle\langle b_j|\phi_l\rangle \tag{2.2.20}$$

Using this and our knowledge that the expectation of a function $\langle\hat{O}\rangle$ can be calculated by taking the trace over the composite system (where $\hat{O} = \hat{O}_A \otimes \hat{I}_B$). Thus we can use the above result to immediately trace over the system B leaving,

$$\langle\hat{O}\rangle = \sum_{k,l}\langle\phi_l|\langle\psi_k|\hat{\rho}(\hat{O}_A \otimes \hat{I}_B)|\psi_k\rangle|\phi_l\rangle \tag{2.2.21}$$

$$= \sum_k \langle\psi_k|\left(\text{Tr}_B(\hat{\rho})\right)\hat{O}_A|\psi_k\rangle \tag{2.2.22}$$

$$= \text{Tr}_A(\hat{\rho}_A\hat{O}_A) \tag{2.2.23}$$

Thus, when we want to work with the measurement statistics regarding those measurements which are only made on the subsystem A then the only thing we need to consider is the reduced-density matrix $\hat{\rho}_A$.

This can be trivially generalised to many dimensions, which is important for our work with decoherence as we will usually work with a system interacting with an environment composed of many different degrees of freedom which are not all available to us, as such we will want to 'trace these out'. An operator $\hat{O}$ acting only on the system 'j' and the identity operator acting on the rest in n-dimensions will be of the form,

$$\hat{I}_1 \otimes \hat{I}_2 \otimes ... \otimes \hat{I}_{j-1} \otimes \hat{O}_j \otimes \hat{I}_{j+1} \otimes ... \otimes \hat{I}_n \tag{2.2.24}$$

which ultimately, analogously to before, leaves

$$\langle\hat{O}\rangle = \text{Tr}_j(\hat{\rho}_j\hat{O}_j) \tag{2.2.25}$$

We now consider the properties of a reduced-density matrix and compare them to those earlier exhibited by pure-state and mixed-state density matrices. Let us begin by considering $\hat{\rho}_A$ of a bipartite system described by the state vector $|\psi\rangle = \sum_i^2 \frac{1}{\sqrt{2}}(|a_i\rangle|b_i\rangle)$ as earlier where we showed this leaves the reduced-density matrix as,

$$\frac{1}{2}(|a_1\rangle\langle a_1| + |a_2\rangle\langle a_2| + |a_1\rangle\langle a_2|\langle b_1|b_2\rangle + |a_2\rangle\langle a_1|\langle b_2|b_1\rangle) \qquad (2.2.26)$$

where normally we cannot guarantee that $|b_1\rangle$ and $|b_2\rangle$ are orthogonal, and even in the case where they are $\mathrm{Tr}_A(\hat{\rho}_A) < 1$ and in our case equals a half. Thus there is a formal similarity between reduced-density matrices and mixed-state density matrices. Indeed, only in the case where the overlap $\langle b_1|b_2\rangle = 1$ do we have the trace equal to unity which is equivalent to the case where the two systems were not entangled in the first place. This formal similarity must not be taken literally, it does NOT mean that reduced-density matrices are equivalent to mixed-state density matrices. In general density matrices are merely a tool for calculating probabilities for measurements performed on states and as such the probability distribution of such a measurement. Thus the formal similarity simply applies to the probability distribution, so do not be fooled into thinking that somehow by interaction with system B, system A has lost its superposition qualities and become an ensemble, our knowledge being changed to 'classical ignorance'. This will be a very important distinction when discussing decoherence later.

2.2.3 Von-Neumann Ideal Measurement Scheme

This section deals with the question of, starting with two distinct states, by which we mean non-entangled states, how can a composite entangled state arise? How is it that two subsystems lose their individuality to become a quantum-mechanical whole? These questions could be split into two distinct parts, firstly the physical issue of what exactly occurs during two states becoming entangled, which we shall effectively ignore and simply say that two systems 'interact' in some manner to become entangled. What we are interested in is the second part to this question, namely the mathematical ways in which two systems 'interact' and emerge as a composite entangled system. This process is often represented in terms of a von-Neumann measurement (which was originally developed in his seminal book of 1932 [29]). The importance of this approach is in treating both system and apparatus as being governed by the laws of quantum mechanics, this marks a radical departure from the Copenhagen interpretation where the apparatus was classical and the system quantum. This new measurement scheme will finally allow us to introduce the basic formalism of quantum decoherence.

Let us begin with a system S in $\mathcal{H}_S$ (usually microscopic) with basis vectors $\{|s_i\rangle\}$ and a (usually macroscopic) measuring apparatus A represented in turn by basis vectors $\{|a_i\rangle\}$ in $\mathcal{H}_A$. It is important to note here that the respective size of system and environment is not actually important (provided $\dim(\mathcal{H}_S) \leq \dim(\mathcal{H}_\epsilon)$) in the sense that it has no relevance to the following argument, however it is reasonable to assume the system is microscopic as we wish to ensure we can create a superposition of the states $\{|s_i\rangle\}$. The purpose of A is to measure the state of S i.e. $|s_i\rangle$ causes system A to move to a state $|a_i\rangle$, having started in some ready state which we shall denote $|a_r\rangle$. Therefore, our interaction looks like

$$|s_i\rangle|a_r\rangle \longrightarrow |s_i\rangle|a_i\rangle \qquad (2.2.27)$$

$\forall i$. Here the initial and final states belong to the tensor product of Hilbert spaces $\mathcal{H}_A \otimes \mathcal{H}_S$ describing the system-environment composite system SA, although we note that currently the system is still separable into two distinct subsystems and as such is not entangled. Our process has effectively established a 1-1 correspondence between states in the system and states in the apparatus. We have also made an assumption here that measurement does not affect the state of the system, this is why it is usually called the von-Neumann ideal measurement scheme, or is equivalently referred to as a quantum non-demolition measurement.

Now thus far there has been no entanglement meaning that the final state is still separable. However, let us begin with a superposition of system states $|\psi\rangle = \sum_i c_i|s_i\rangle$ which means our measurement is of the form,

$$|\psi\rangle|a_r\rangle = \left(\sum_i c_i|s_i\rangle\right)|a_r\rangle \longrightarrow \sum_i c_i|s_i\rangle|a_i\rangle \qquad (2.2.28)$$

Where this evolution represents the ideal von-Neumann quantum measurement scheme. Inspection of the right-hand side will show that generally (i.e., when more than one $c_i \neq 0$) we have a resulting state which is entangled, thus we have dynamically created entanglement. What has in effect happened here is not measurement in the conventional sense, indeed it is not obvious that a measurement has occurred at all, what has happened is that the superposition originally present only at the level of the system has been 'amplified' to the level of the system-apparatus composite. The fact that no measurement has explicitly occurred is the reason why this final state is often referred to as pre-measurement. There is one key way in which at first glance this 'measurement-scheme' seems to violate our known properties of quantum-mechanics, this problem results from a fundamental basis-ambiguity in the measurement scheme.

Let us first assume that the $|a_i\rangle$ are mutually orthogonal such that we do indeed have an unambiguous measurement with regard to the apparatus (which is why we require our condition on the dimensions). Now we can show that unless all c_i are distinct then we can achieve a result which apparently defies quantum-mechanics. As an example, consider both the system and apparatus as described by spin-$\frac{1}{2}$ particles and as is customary we will consider them in the z-direction. If we

set up one of the Bell-states as mentioned in the previous chapter with the system becoming entangled with the apparatus in such a way that the apparatus exactly mirrors the system,

$$\frac{1}{\sqrt{2}}(|1_z\rangle + |0_z\rangle))|a_r\rangle \longrightarrow \frac{1}{\sqrt{2}}(|1_z\rangle|1_z\rangle + |0_z\rangle|0_z\rangle) \tag{2.2.29}$$

which behaves as we expect. However, let us consider a change of basis into the spin-x direction where we know from last chapter the eigenvectors in the z-direction expressed in the x-direction are:

$$|0_z\rangle = \frac{1}{\sqrt{2}}(|0_x\rangle + |1_x\rangle) \tag{2.2.30}$$

$$|1_z\rangle = \frac{1}{\sqrt{2}}(|0_x\rangle - |1_x\rangle) \tag{2.2.31}$$

which means that if we change basis in both system and apparatus we get:

$$\begin{aligned}
\frac{1}{\sqrt{2}}\left(|1_z\rangle|1_z\rangle + |0_z\rangle|0_z\rangle\right) &= \frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{2}}\left(|0_x\rangle - |1_x\rangle\right)|1_z\rangle + \frac{1}{\sqrt{2}}\left(|0_x\rangle + |1_x\rangle\right)|0_z\rangle\right) \\
&= \frac{1}{\sqrt{2}}\left(\frac{1}{2}\left(|0_x\rangle - |1_x\rangle\right)\left(|0_x\rangle - |1_x\rangle\right) + \frac{1}{2}\left(|0_x\rangle + |1_x\rangle\right)\left(|0_x\rangle + |1_x\rangle\right)\right) \\
&= \frac{1}{\sqrt{2}}\left(|0_x\rangle|0_x\rangle + |1_x\rangle|1_x\rangle\right) \tag{2.2.32}
\end{aligned}$$

And as such, if we interpret this in the spirit of the von-Neumann measurement scheme, this would illustrate that the apparatus has simultaneously 'measured' spin of the system in both the x- and z-direction. Since these are non-commuting observables in the standard formalism we know that this is not allowed by the laws of quantum mechanics.

This problem is resolved if we consider looking at what our final line would look like as a process,

$$\frac{1}{\sqrt{2}}(|1_x\rangle + |0_x\rangle))|a_r\rangle \longrightarrow \frac{1}{\sqrt{2}}(|1_x\rangle|1_x\rangle + |0_x\rangle|0_x\rangle) \tag{2.2.33}$$

but, the left-hand side of this equation is simply equal to $|0_z\rangle$ and thus, by the dynamics described originally, this state does not in fact become entangled with the environment at all. Essentially what we are saying here is that the dynamics described in (2.2.27) and (2.2.28) are not directly transcribable into other bases. This immediately indicates in what way information about spin in the x-direction is not encoded by the environment, since after interaction and a change of basis for the system the system is,

$$\frac{1}{\sqrt{2}}\left(\frac{1}{\sqrt{2}}\left(|0_x\rangle - |1_x\rangle\right)|1_z\rangle + \frac{1}{\sqrt{2}}\left(|0_x\rangle + |1_x\rangle\right)|0_z\rangle\right) \tag{2.2.34}$$

As such, any measurement on the environment in the basis of $\{|0_z\rangle, |1_z\rangle\}$ cannot distinguish between $|0_x\rangle$ and $|1_x\rangle$ as we would subsequently have equal chance of measuring $|0_x\rangle$ as $|1_x\rangle$. Physically, it is easier to visualise: in order to measure a different spin direction we would have to rotate the apparatus and as such change the dynamics of interaction between the apparatus and system. Therefore it is the nature of the interaction as described by (2.2.28) that selects the so-called 'preferred-basis' for our measurements, and once this interaction is specified it fixes what information the apparatus can encode about the system under scrutiny.

2.3   Introduction to Decoherence

Until this point, the complementarity between which-path information versus interference has been discontinuous, that is we have considered something either as a particle or a wave, let us now consider partial which-path information so that we have a cross between particle and wave characteristics. Because of this we break with wavefunction collapse which is, by nature, discontinuous so we will instead use our notation of density matrices. Let us consider the double-slit experiment where we have two orthonormal kets, $|\psi_1\rangle$ and $|\psi_2\rangle$ which represent the particle travelling through slit 1 and slit 2 respectively. Thus, if we were to imagine an apparatus that measures through which of the two slits the particle passed, the dynamics of this process in our von-Neumann notation would be:

$$|\psi_1\rangle|r\rangle \longrightarrow |\psi_1\rangle|1\rangle$$

$$|\psi_2\rangle|r\rangle \longrightarrow |\psi_2\rangle|2\rangle \tag{2.3.1}$$

as might be expected. If we were to construct a superposition of these states and evolve them by an interaction with the environment then we would have,

$$\frac{1}{\sqrt{2}}(|\psi_1\rangle + |\psi_2\rangle)|r\rangle \longrightarrow \frac{1}{\sqrt{2}}(|\psi_1\rangle|1\rangle + |\psi_2\rangle|2\rangle) = |\psi\rangle \tag{2.3.2}$$

We now consider the density matrix of this state $|\psi\rangle$,

$$\hat{\rho} = |\psi\rangle\langle\psi| \qquad (2.3.3)$$

We trace over the apparatus states to obtain the reduced density matrix of the system $\hat{\rho}_S$ which is given by,

$$\hat{\rho}_S = \sum_{x=1,2} \langle x|\rho|x\rangle = \frac{1}{2}|\psi_1(x)|^2 + \frac{1}{2}|\psi_2(x)|^2 + Re\left\{\psi_1(x)\psi_2^*(x)\langle 2|1\rangle\right\} \qquad (2.3.4)$$

where $\psi_i(x)$ is defined as $\langle x|\psi_i\rangle$ for $i = 1, 2$. In the two limiting scenarios we see that we recover our previous results, $\langle 2|1\rangle = 0$ will give us the particle regime, whereas $\langle 2|1\rangle = 1$ gives us the wave scenario. Physically we are saying that if $|1\rangle$ and $|2\rangle$ are entirely distinct then we have complete wavefunction collapse and our results verify this, conversely if $|1\rangle$ and $|2\rangle$ are completely indistinguishable, i.e. $|1\rangle = |2\rangle$ then we have no 'which-path' information and as expected the results are those which represent the wave scenario. However, in the general intermediate case, we see that an increase in which-path information, which is shown by increasing distinguishability between the two states of the apparatus, cause the off-diagonal elements of the reduced-density matrix to decrease.

The degree to which an interference pattern can be observed is determined by the available which-path information encoded in some system entangled with the system of interest, and this amount can be changed without necessarily influencing the spatial wave function of the object itself. We now inquire as to what exactly we mean by our measuring apparatus? The photons striking this page here are continually carrying away information about the position of the letters on the page and as such could be considered a measuring apparatus for the spatial position of this page and its contents. So we shall from now on consider the environment as our measuring apparatus which encodes information about our system of interest by becoming entangled with it. We showed earlier that the form of this interaction determines the preferred observables, if we consider that on a macroscopic scale most interaction terms in a Hamiltonian are a function of distance, such as the inverse square law or Coulomb potential etc. As such the environment 'selects' preferred observables which is often called "Einselection" or "superselection" of pointer-states. In comparison to this if we consider a closed microscopic system, such as a Hydrogen atom, we know that the Hamiltonian has eigenstates which are Energy eigenstates, as such without any interaction it is these states which are "selected" to be the preferred physical quantities. It should be clear from this discussion that the form of the preferred observable is a result of those states which are least affected by the Hamiltonian. It is unlikely in a non-closed system that we will be able to find exact diagonal states, so the preferred physical quantity will be a compromise between the eigenstates of the interaction term, usually position and the eigenstates of the self-Hamiltonian, meaning energy.

We now consider again our reduced-density matrix but with slightly different notation representing the environment instead of an abstract apparatus. We say,

$$\hat{\rho}_{\text{particle}} = \frac{1}{2}\left\{|\psi_1\rangle\langle\psi_1| + |\psi_2\rangle\langle\psi_2| + |\psi_1\rangle\langle\psi_2|\langle E_1|E_2\rangle + |\psi_2\rangle\langle\psi_1|\langle E_2|E_1\rangle\right\} \qquad (2.3.5)$$

where we have written out (2.3.4) fully and replaced $|1\rangle \longrightarrow |E_1\rangle$ and similarly $|2\rangle \longrightarrow |E_2\rangle$. In (2.3.5) we see that the last two terms represent interference between the two slits, thus we see that if $\langle E_1|E_2\rangle \longrightarrow 0$ then the interference terms are suppressed and the corpuscular-view emerges. This physically says that: as the system interacts with the environment in such a way that the environmental states representing $|\psi_1\rangle$ and $|\psi_2\rangle$ become increasingly distinguishable causing the overlap to diminish, then the interference terms are suppressed. The interference is still present at a 'global' level of the system-environment, but is suppressed at the 'local' level of the system as described by the reduced-density matrix. This suppression of local phase coherence by interaction with an environment of some sort is called decoherence, where we recall that by phase coherence we mean the well-defined phase relations between the components in the superposition.

Once again it is worth stressing the nature of this decoherence, we cannot ensure that the effect of interaction between system and environment will actually result in distinguishable environments and as such the dynamics of the interaction, as we have seen before, is all important. We might not expect the scattering of photons on a particle to resolve a superposition in energy eigenstates however we would expect it to cause rapid decoherence in the position basis. This brings to an end our very simplistic and general introduction to the notion of decoherence, we shall now see an example of a model of decoherence in order that we might better understand the physical and the mathematical aspects of the process.

2.4 Summary

- The standard operator formalism of quantum mechanics leaves several gaps which have been grouped slightly misleadingly under the term 'measurement problem'. These essentially ask how we obtain classical results from underlying quantum behaviour, the most important part of this for us being the emergence of single quantities in the macroscopic limit rather than superpositions.

- we defined pure-state density matrices as $\hat{\rho} \equiv |\psi\rangle\langle\psi|$ which acts as a projection operator onto the state $|\psi\rangle$.

- We introduced the trace operation defined by $Tr(\hat{\rho}) = \sum_i \langle\phi_i|\hat{\rho}|\phi_i\rangle$. This operation has several important relations which it satisfies such as invariance under cyclic permutations, ($\text{Tr}(\hat{A}\hat{B}\hat{C}) = \text{Tr}(\hat{C}\hat{A}\hat{B})$ etc.) and linearity ($\text{Tr}(x\hat{A} + y\hat{B}) = x\text{Tr}\hat{A} + y\text{Tr}\hat{B}$). We also noted that we could use the trace operation to find expectation values for observables through the relation $\text{Tr}(\hat{\rho}\hat{O}) = \sum_i o_i|\langle o_i|\psi_i\rangle|^2 = \langle\hat{O}\rangle$.

- We then introduced the partial trace which acts on entangled states, we started with a pure state density matrix of an entangled state with $\sum_{i,j}^2 \frac{1}{2}(|a_i\rangle\langle a_j| \otimes |b_i\rangle\langle b_j|)$ and then we trace over only the B-system. $\mathrm{Tr}_B(\hat{\rho}) = \hat{\rho}_A = \frac{1}{2}\sum_l \sum_{i,j}^2 |a_i\rangle\langle a_j|\langle\phi_l|b_i\rangle\langle b_j|\phi_l\rangle$, which by completeness $= \frac{1}{2}\sum_{i,j}|a_i\rangle\langle a_j|\langle b_j|b_i\rangle$.

- We introduced the von-Neumann ideal measurement scheme which took the form $\frac{1}{\sqrt{2}}(|1\rangle + |2\rangle)|E_r\rangle \longrightarrow \frac{1}{\sqrt{2}}(|1\rangle|E_1\rangle + |2\rangle|E_2\rangle)$ where the form of the interaction completely determines the preferred states.

- We then use our earlier partial trace to obtain $\hat{\rho}_S = \mathrm{Tr}_\varepsilon\hat{\rho} = \mathrm{Tr}_\varepsilon\left(\frac{1}{\sqrt{2}}(\sum_{i=1,2}|i\rangle\langle j| \otimes |E_i\rangle\langle E_j|)\right)$. Once evaluated this gives,

$$\frac{1}{2}(|1\rangle\langle 1| + |2\rangle\langle 2| + |1\rangle\langle 2|\langle E_1|E_2\rangle + |2\rangle\langle 1|\langle E_2|E_1\rangle)$$

from which it is clear that as $\langle E_1|E_2\rangle \longrightarrow 0$ spatial coherences are locally suppressed, where by locally we mean on the level of the reduced density matrix for the system but not on the system-environment composite. In this sense we say that the environment 'measures' the system, and produces single states from superpositions. This is the process known as decoherence.

3 Scattering Model

In this chapter we are going to develop a simple model for decoherence which is usually referred to as 'The Scattering Model'. During this derivation we will encounter many of the key notions, assumptions and simplifications which typify models for decoherence. Ultimately our aim here is to obtain values whichare justified in representing decoherence under certain restrictions in order that we can appreciate the dynamics and timescales of decoherence. This chapter very closely follows the model as derived in Chapter.3 of [26], which is a fantastic introduction to the subject. The material is similar, Schlosshauer however considers a wider range of material and not always in so much depth.

3.1 Basic Construction of Our Scattering Model

We now construct a model in order that we may demonstrate the rate of decoherence we can expect to experience in "normal" circumstances, by which we mean on a macroscopic (or at least mesoscopic) scale. We consider an object (the system S) that scatters a collection of other particles (the environment ε). We make the standard assumption that S and ε are initially completely uncorrelated, i.e. the pure-state density matrix $\hat{\rho}$ is of a separable form

$$\hat{\rho}(0) = \hat{\rho_S}(0) \otimes \hat{\rho_\varepsilon}(0) \tag{3.1.1}$$

Let us initially consider the effect on the density matrix of a single scattering event, then later generalise this to a greater number of events.

We denote the initial state of our system with centre-of-mass location x by a position eigenstate $|x\rangle$, and $|\phi_i\rangle$ denoting the initial state of the incoming environmental particle. Then the scattering event we express through the scattering operator $\hat{S}$ (the so-called "S-matrix") acting on the initial state,

$$|x\rangle|\phi_i\rangle \rightarrow \hat{S}\left(|x\rangle|\phi_i\rangle\right) \tag{3.1.2}$$

where we have used the separability assumption for the initial state. The state $|x\rangle$ can be expressed as the state $|x = 0\rangle$ (corresponding to the scattering centre being locate at the origin) translated by the momentum operator $\hat{p}$ of the system, $|x\rangle = e^{-i\hat{p}\cdot x/\hbar}|x = 0\rangle$ implementing this into (3.1.2) gives,

$$e^{-i\hat{p}\cdot x/\hbar}|0\rangle|\phi_i\rangle \longrightarrow \hat{S}e^{-i\hat{p}\cdot x/\hbar}|0\rangle|\phi_i\rangle = \hat{S}e^{-i(\hat{p}+\hat{q})\cdot x/\hbar}|0\rangle e^{i\hat{q}\cdot x/\hbar}|\phi_i\rangle. \tag{3.1.3}$$

Here, we have denoted the momentum operator for the scattered particle as $\hat{q}$, and thus $\hat{P} \equiv \hat{p} + \hat{q}$ is the momentum operator for the Sε composite.

If we now implement the assumption that the scattering interaction is invariant if we were to translate the joint system in space (i.e. invariant under translations generated by $\hat{P}$, physically a perfectly reasonable requirement), meaning $[\hat{S}, \hat{P}] = 0$. This allows us to pull the first exponential on the right-hand side of our latest evolution equation (3.1.3) to the front and obtain,

$$\hat{S}\left(|x\rangle|\phi_i\rangle\right) = e^{-i(\hat{p}+\hat{q})\cdot x/\hbar}\hat{S}|0\rangle e^{i\hat{q}\cdot x/\hbar}|\phi_i\rangle \tag{3.1.4}$$

To proceed further, a key assumption is made, we add the requirement that interaction between the environment and the particle leads to negligible recoil of the object. This essentially means that the particle remains spatially undisturbed by the scattering event, the consequences therefore being limited to the creation of entanglement between the system and the environment. We interpret this, in light of the von-Neumann measurement scheme, as a measurement of the system by the environment.

Our last assumption is justifiable provided the mass of the scattering system is much greater than that of the scattered particle, such that recoil effects can be ignored, (Note that when we generalise this to many particles being scattered such an assumption will have to be strengthened. A single electron scattering off a water molecule is negligible, but many may have a significant effect). As such, in our cases of interest, namely the mesoscopic and macroscopic scales, this assumption is physically reasonable. However situations where the masses of the scattering system and scattered particles are closer, this assumption is not physically realistic.

For the following derivation, this no-recoil assumption is useful since the result is that the S-matrix acting on the composite system-environment state, affects only the scattering particles and not the state of the system. We can therefore update our earlier evolution equation,

$$\begin{aligned} \hat{S}\left(|x\rangle|\phi_i\rangle\right) &= e^{-i(\hat{p}+\hat{q})\cdot x/\hbar}|0\rangle \hat{S}_0 e^{i\hat{q}\cdot x/\hbar}|\phi_i\rangle \\ &= e^{-i\hat{p}\cdot x/\hbar}|0\rangle e^{-i\hat{q}\cdot x/\hbar}\hat{S}_0 e^{i\hat{q}\cdot x/\hbar}|\phi_i\rangle \\ &= |x\rangle e^{-i\hat{q}\cdot x/\hbar}\hat{S}_0 e^{i\hat{q}\cdot x/\hbar}|\phi_i\rangle \end{aligned} \tag{3.1.5}$$

Where we added a subscript "0" to the scattering operator $\hat{S}$ which indicates that this operator refers specifically to a scattering process where the scattering centre is at the origin. We use the last line of this equation to define the translated scattering operator

$$\hat{S}_x \equiv e^{-i\hat{q}\cdot x/\hbar}\hat{S}_0 e^{i\hat{q}\cdot x/\hbar} \tag{3.1.6}$$

This operator now describes the scattering process where the scattering centre is at position x. Therefore, the scattering process is given as:

$$|x\rangle|\phi_i\rangle \longrightarrow \hat{S}|x\rangle|\phi_i\rangle = |x\rangle\hat{S}_x|\phi_i\rangle \equiv |x\rangle|\phi(x)\rangle \tag{3.1.7}$$

where we have introduced the notation $|\phi(x)\rangle$ for the final state of the environmental particle scattered at x. It is now plain how in our earlier notation this last equation parallels the von-Neumann scheme for ideal measurement, namely we have described an interaction which results in the environmental state varying, depending on some property of the system. As such, we interpret this as a measurement like interaction where correlations are established between the state $|x\rangle$, and the final state $|\phi(x)\rangle$ of the particle, which in this way encodes information about the location of the scattering centre, provided $\langle\phi(x)|\phi(x')\rangle \rightarrow 0$ for $x \neq x'$.

If we now transcribe our results into the density operator notation then the initial density matrix is given by,

$$\hat{\rho}(0) = \hat{\rho}_S(0) \otimes \hat{\rho}_\varepsilon(0) = \int dx \int dx' \rho_S(x,x',0)|x\rangle\langle x'| \otimes |\phi_i\rangle\langle\phi_i| \tag{3.1.8}$$

Where as a result of changing from discrete to continuous variables we have made a transition from using sums to using integrals. After the action of $\hat{S}_x$ we have,

$$\int dx \int dx' \rho_S(x,x',0)|x\rangle\langle x'| \otimes |\phi(x)\rangle\langle\phi(x')| \tag{3.1.9}$$

We now trace over the environment to obtain our reduced density matrix $\hat{\rho}_S$, If we express the environment as a complete set of orthonormal eigenstates $|a\rangle$ which are continuous (since our environment consists of harmonic oscillators), then simply considering the pertinent part of equation (3.1.9), we have

$$\int da\langle\phi(x')|a\rangle\langle a|\phi(x)\rangle = \langle\phi(x')|\phi(x)\rangle \tag{3.1.10}$$

where in this last equality we have used completeness of our basis $|a\rangle$. This leaves a reduced density matrix

$$\hat{\rho}_S = \text{Tr}_\varepsilon\hat{\rho} = \int dx \int dx' \rho_S(x,x',0)|x\rangle\langle x'|\langle\phi(x')|\phi(x)\rangle \tag{3.1.11}$$

Which, by expressing in the position basis, we can therefore summarize as, $\rho_S(x,x',0) \longrightarrow \rho_S(x,x',0)\langle\phi(x')|\phi(x)\rangle$. We note that the local suppression of spatial coherence resulting from the scattering event, is entirely expressed by the overlap $\langle\phi(x')|\phi(x)\rangle$ of the relative final states of the scattered particles. We now endeavour to calculate the time dependence of this overlap, remembering that ideally we would like the overlap to decay over time in order that the scattering event should act like a measurement.

3.2   Calculating the Decoherence Factor

To proceed, we express the scattering operator $\hat{S}_0$ in terms of another operator $\hat{T}$ (the "T-matrix") as:

$$\hat{S}_0 = \hat{I} + i\hat{T} \tag{3.2.1}$$

The reason for this substitution, is that we may define $\hat{T}$ in such a way that the elements of the T-matrix as described in the momentum eigenbasis $\{|q\rangle\}$ of the scattered particle have the convenient property of being defined in terms of the scattering amplitude, which we here denote as,

$$\langle q|\hat{T}|q'\rangle = \frac{i}{2\pi\hbar q}\delta(q - q')f(q,q') = \frac{i}{2\pi\hbar m}\delta(E - E')f(q,q') \tag{3.2.2}$$

Where m is the mass of the environmental particle and $q = |\vec{q}|$. The term $\delta(E - E')$ ensures energy conservation which is required by the assumption of recoil-free elastic scattering. This in turn is useful since, $|f(q,q')|^2$ is an experimentally accessible quantity i.e. the differential cross section $\frac{d\sigma}{d\Omega}$ for the scattering process, which is defined as

$$\frac{d\sigma}{d\Omega} \equiv \frac{\text{scattered flux}}{\text{incident flux}} \tag{3.2.3}$$

Since the scattering operator $\hat{S}_0$ is unitary, we have the relation, $\hat{S}_0\hat{S}_0^\dagger = \hat{I}$. Substituting our expression for $\hat{S}_0$ in terms of $\hat{T}$ here, we obtain a relation in $\hat{T}$, namely

$$(\hat{I} + i\hat{T})(\hat{I} + i\hat{T})^\dagger = \hat{I} \longrightarrow \hat{T}\hat{T}^\dagger + i(\hat{T} - \hat{T}^\dagger) = 0 \tag{3.2.4}$$

This result will be useful later on.

Using the expression (3.1.7) for the environmental states, we can trivially write the overlap $\langle\phi(x')|\phi(x)\rangle$ as

$$\langle\phi(x')|\phi(x)\rangle = \langle\phi_i|\hat{S}_x^\dagger\hat{S}_x|\phi_i\rangle \tag{3.2.5}$$

In standard quantum mechanics notation, this is equivalent to asking the expectation value of the product $\hat{S}_x^\dagger \hat{S}_x$ which are the translated scattering operators (3.1.6) in the (pure) state $|\phi_i\rangle$. If we use the trace rule, as introduced in the last chapter, we write this same expression as,

$$\langle \phi(x')|\phi(x)\rangle = Tr_\varepsilon\{\hat{\rho}_\varepsilon(0)\hat{S}_x^\dagger \hat{S}_x\} \tag{3.2.6}$$

with $\hat{\rho}_\varepsilon(0) = |\phi_i\rangle\langle\phi_i|$. This is the expression of interest that we shall now endeavour to evaluate. Let us assume that the particle is restricted to a box-normalization volume V, requiring eigenstates $|\tilde{q}\rangle$ which are normalized over the volume V,

$$|\tilde{q}\rangle \equiv \left(\frac{(2\pi\hbar)^3}{V}\right)^{\frac{1}{2}} |q\rangle \tag{3.2.7}$$

These kets $|\tilde{q}\rangle$ form a complete orthonormal basis over V such that $\sum_q |\tilde{q}\rangle\langle\tilde{q}| = \hat{I}_V$ with $\tilde{q} \in Q_V$, where Q_V is the set of all momenta which fulfill periodic boundary conditions in the volume V, and $\hat{I}_V$ denotes the identity in this space of wavefunctions defined by Q_V.

We now express the initial density matrix $\hat{\rho}_\varepsilon(0)$ of the environmental particle in terms of the normalized momentum eigenstates $|\tilde{q}\rangle$,

$$\hat{\rho}_\varepsilon(0) = \frac{(2\pi\hbar)^3}{V} \sum_{q\in Q_V} \mu(q)|\tilde{q}\rangle\langle\tilde{q}|, \tag{3.2.8}$$

where $\mu(q)$is the momentum-space density. As mentioned the great advantage of using this expansion is that $\hat{T}$ is diagonal in $\{|q\rangle\}$, therefore also in the properly normalized V-volume basis $\{|\tilde{q}\rangle\}$.

This now permits us to evaluate $\langle \phi(x')|\phi(x)\rangle$, see (3.2.6). Using the expansion (3.2.8) for the state of the environment, we get:

$$\langle \phi(x')|\phi(x)\rangle = \frac{(2\pi\hbar)^3}{V} \sum_{q\epsilon Q_V} \mu(q)\langle\tilde{q}|\hat{S}_x^\dagger \hat{S}_x|\tilde{q}\rangle$$

$$= \frac{(2\pi\hbar)^3}{V} \sum_{q\epsilon Q_V} \mu(q)\langle\tilde{q}|e^{-i\hat{q}\cdot x'/\hbar}\hat{S}_0^\dagger e^{-i\hat{q}\cdot(x-x')/\hbar}\hat{S}_0 e^{i\hat{q}\cdot x/\hbar}|\tilde{q}\rangle$$

$$= \frac{(2\pi\hbar)^3}{V} \sum_{q\epsilon Q_V} \mu(q)e^{iq\cdot(x-x')/\hbar}\langle\tilde{q}|\hat{S}_0^\dagger e^{-i\hat{q}\cdot(x-x')/\hbar}\hat{S}_0|\tilde{q}\rangle \tag{3.2.9}$$

Now we use the relation (3.2.1) i.e. $\hat{S}_0 = \hat{I} + i\hat{T}$ and insert this into equation (3.2.9) and continue by noting the relation (3.2.4), giving

$$\langle \phi(x')|\phi(x)\rangle = \frac{(2\pi\hbar)^3}{V} \sum_{q\epsilon Q_V} \mu(q)e^{i\hat{q}\cdot(x-x')/\hbar}\langle\tilde{q}|(\hat{I} - i\hat{T}^\dagger)e^{-i\hat{q}\cdot(x-x')/\hbar}(\hat{I} + i\hat{T})|\tilde{q}\rangle$$

$$= \frac{(2\pi\hbar)^3}{V} \sum_{q\epsilon Q_V} \mu(q)\{1 - \langle\tilde{q}|\hat{T}\hat{T}^\dagger|\tilde{q}\rangle + e^{i\hat{q}\cdot(x-x')/\hbar}\langle\tilde{q}|\hat{T}^\dagger e^{-i\hat{q}\cdot(x-x')/\hbar}\hat{T}|\tilde{q}\rangle\} \tag{3.2.10}$$

Here we can remove all exponentials in the second term since the momentum observable commutes with the identity matrix, before we use (3.2.4).

Let us first turn our attention to the second and third term in the last line of (3.2.10) by inserting a complete set of momentum eigenstates $|\tilde{q}\rangle$,

$$\langle\tilde{q}|\hat{T}\hat{T}^\dagger|\tilde{q}\rangle = \langle\tilde{q}|\hat{T}|\tilde{q}\rangle\langle\tilde{q}|\hat{T}^\dagger|\tilde{q}\rangle = |\langle\tilde{q}|\hat{T}|\tilde{q}\rangle|^2 \tag{3.2.11}$$

So substituting this gives,

$$\langle \phi(x')|\phi(x)\rangle = \frac{(2\pi\hbar)^3}{V} \sum_{q\epsilon Q_V} \mu(q)\{\hat{I} - \sum_{q\epsilon Q_V} (1 - e^{i(\hat{q}-\hat{q}')\cdot(x-x')/\hbar})|\langle q|\hat{T}|q'\rangle|^2\} \tag{3.2.12}$$

Where q' is defined as the eigenvalue to $\hat{T}|\tilde{q}\rangle$. We proceed in the continuum limit of momentum states $|\tilde{q}\rangle$ by replacing the sum by an integral. We use the standard transformation relation

$$\frac{(2\pi\hbar)^3}{V} \sum_{q\epsilon Q_V} \longrightarrow \int dq \tag{3.2.13}$$

We also use that $\int dq\mu(q) = 1$ and employ definition (3.2.7), to change equation (3.2.12) into

$$\langle \phi(x')|\phi(x)\rangle = 1 - \int dq\mu(q)\frac{(2\pi\hbar)^3}{V} \int dq'(1 - e^{i(\hat{q}-\hat{q}')\cdot(x-x')/\hbar})|\langle q|\hat{T}|q'\rangle|^2 \tag{3.2.14}$$

We now use a parameter T, which is used to denote the time passing in the scattering process. This allows us to use (3.2.14), to express the evolution of the reduced density matrix as

$$\rho_S(x, x', T) - \rho_S(x, x', 0) = -\rho_S(x, x', 0) \int dq \mu(q) \frac{(2\pi\hbar)^3}{V} \int dq'(1 - e^{i(\hat{q}-\hat{q}')\cdot(x-x')/\hbar})|\langle q|\hat{T}|q'\rangle|^2 \tag{3.2.15}$$

It is important to note that in writing (3.2.15), we have made the implicit assumption that the characteristic timescale for the free evolution of the system is much longer than the average time between scattering events, such that the change of the density matrix during the interval T not due to the scattering process is negligible, i.e. the self-Hamiltonian of the system $\hat{H}_S$ is has a timescale $\tau_{\text{evol}} \gg \tau_{\text{deco}}$.

Next we consider the squared matrix element $|\langle q|\hat{T}|q'\rangle|^2$ in our equation. We use the form

$$\langle q|\hat{T}|q'\rangle = \frac{i}{2\pi\hbar m}\delta(E - E')f(q, q') \tag{3.2.16}$$

from (3.2.2), which leads to the relation

$$|\langle q|\hat{T}|q'\rangle|^2 = \frac{1}{(2\pi\hbar m)^2}\delta^2(E - E')|f(q, q')|^2 \tag{3.2.17}$$

we interpret $|\langle q|\hat{T}|q'\rangle|^2$ in the standard manner, as the probability of making a scattering induced transition $|q\rangle \longrightarrow |q'\rangle$.

With regard to the squared energy delta function we consider the energy delta function in its Fourier-integral representation

$$\delta(E - E') = \lim_{T\to\infty} \frac{1}{2\pi\hbar} \int_{-T/2}^{T/2} e^{i(E-E')t/\hbar}dt \tag{3.2.18}$$

Substituting this in leaves,

$$\begin{aligned}
\delta^2(E - E') &= \delta(E - E') \lim_{T\to\infty} \frac{1}{2\pi\hbar} \int_{-T/2}^{T/2} e^{i(E-E')t/\hbar}dt \\
&= \delta(E - E') \lim_{T\to\infty} \frac{1}{2\pi\hbar} \int_{-T/2}^{T/2} dt \\
&= \delta(E - E') \lim_{T\to\infty} \frac{T}{2\pi\hbar}
\end{aligned} \tag{3.2.19}$$

where the second line follows from the action of the δ-function on the exponential, meaning the integral vanishes unless E = E'.

The time-parameter T therefore clearly represents the interval of time wherein the interaction is "activated". Equation (3.2.19) then shows the transition probability growing approximately linearly with T for sufficiently large T. As such allowing T to represent a time interval significantly longer than the typical timescale which we would require if we wanted to limit interaction to a single interaction event occurring, we can write (3.2.19) as

$$\delta^2(E - E') = \delta(E - E')\frac{T}{2\pi\hbar} = \delta(q - q')\frac{m}{q}\frac{T}{2\pi\hbar} \tag{3.2.20}$$

We shall assume that T is shorter than the decoherence timescale of the system resulting from a large number of particles being scattered. Such a region of definition for T is reasonable, as we would intuitively anticipate that in general a high number of collisions would be required to result in a significant degree of spatial decoherence.

We now use (3.2.20) in (3.2.17) and insert the resulting expressions into (3.2.15). The delta-function $\delta(q-q')$ into (3.2.20) ensures that momentum is conserved, meaning $|q'| = |q|$. If we now change $dq' \equiv q^2 d\hat{n}'$, where $d\hat{n}'$ is a solid-angle differential in momentum space, we have

$$\rho_S(x, x', T) - \rho_S(x, x', 0) = -\rho_S(x, x', 0)\frac{T}{V} \int dq \mu(q) v(q) \int d\hat{n}'(1 - e^{i(q-q\hat{n}')\cdot(x-x')/\hbar})|f(q\hat{n}, q\hat{n}')|^2 \tag{3.2.21}$$

Here $v(q)$ denotes the speed of particles with momentum q meaning scattering of massive particles requires $v(q) = q/m$, while photons and other massless particles use $v(q) = c$, with c representing the speed of light.

Equation (3.2.21) represents only a single particle being scattered. if we were to consider a collection of N independent scattering events we would modify our equation by multiplying the integral on the right hand side of (3.2.21) by N. Where of course N/V is the total number density of environmental particles. We simplify this by the assumption that the density of incoming particles is isotropically distributed in space, meaning every initial direction $q/|q|$ is equally likely. This leaves the momentum probability distribution $\mu(q)$ in the form

$$\mu(q) \equiv \frac{1}{4\pi}\left(\frac{N}{V}\right)^{-1} \varrho(q)dqd\hat{n}, \tag{3.2.22}$$

the prefactor is assigned in such a way that (recalling that $\int dq \mu(q) = 1$) $\int dq \varrho(q) = N/V$ which would lead to the instinctive interpretation that $\varrho(q)$ is the number density of incoming particles with magnitude of momentum equal to q.

We divide (3.2.21) by T take the differential limit of small T, and as such obtain our final result for the time-evolution of the reduced density matrix

$$\frac{\partial \rho_S(x, x', t)}{\partial t} = -F(x - x') \rho_S(x, x', t) \tag{3.2.23}$$

the factor $F(x - x')$ Therefore being interpreted as a 'decoherence factor', and given by

$$F(x - x') = \int dq \varrho(q) \upsilon(q) \int \frac{d\hat{n} d\hat{n}'}{4\pi} (1 - e^{iq(\hat{n} - \hat{n}') \cdot (x - x')/\hbar}) |f(q\hat{n}, q\hat{n}')|^2 \tag{3.2.24}$$

(3.2.23) shows that $F(x - x')$ plays the role of a "localization rate", i.e. it's the characteristic decoherence rate for spatial coherences between two positions x and x' to become 'locally' suppressed.

Equations (3.2.23) and (3.2.24) are our primary result, we have found an expression that quantitatively represents the influence of a collection of incoming particles which scatter as a result of our system of interest under a set of seemingly reasonable assumptions. As we might expect, these suppress the interference (off-diagonal) terms in the position density matrix of the object. Until we find a form for the scattering cross-section $|f(q\hat{n}, q\hat{n}')|^2$, our expression is clearly very general.

We now work towards particular numerical examples of the unknown quantitates in (3.2.24) by which we hope to indicate the timescales involved. To prevent us selecting unsuitable situations, let us first quickly review which assumptions were made for our derivation in order that we might bear these in mind as we continue:

1. There are no initial correlations between the system and environment, (this assumption is made in the vast majority of decoherence models).

2. The scattering interaction is invariant under translations of the system-environment composite.

3. The centre-of-mass state of the object is not disturbed by the scattering process.

4. The rate of scattering is much faster than the characteristic evolution timescale of the state of the system induced by the system's self-Hamiltonian.

5. The distribution of the different directions of the incoming particles is isotropic.

3.3 The Long Wavelength Limit

Let us consider the case where the typical wavelength λ_0 of the incoming particle is much longer than the coherent separation $\Delta x = |x - x'|$. This wouldmean that any individual scattering event would fail to result in a resolution of the separation Δx and will therefore carry away an insufficient amount of information to cause complete wavefunction collapse. With this we hope to establish an upper bound on our typical decoherence timescale (equivalently a lower bound on our decoherence rate). We anticipate that a large number of scattering events will be required to create a significant change in the coherent superposition.

So given our assumption $\lambda_0 \gg x_0$ (or equivalently, $q_0 \Delta x/\hbar \ll 1$ for a typical value q_0 of momentum), we look at the effect on $F(x - x')$, see (3.2.24). We first expand the exponential in (3.2.24) up to second order (beyond here we discard the terms since they become negligible), in the argument $q(\hat{n} - \hat{n}') \cdot (x - x')$, i.e.,

$$1 - e^{iq(\hat{n} - \hat{n}') \cdot (x - x')/\hbar} \approx -\frac{i}{\hbar} q(\hat{n} - \hat{n}') \cdot (x - x') + \frac{1}{2!\hbar^2} q^2 ((\hat{n} - \hat{n}') \cdot (x - x'))^2 + 0\left(\frac{q\Delta x}{\hbar}\right)^3 \tag{3.3.1}$$

If we realise that the first term here (indeed all odd powers of $(\hat{n} - \hat{n}') \cdot (x - x')$) fail to contribute to the integral in the expression for $F(x - x')$, see (3.2.24). this can be deduced, since $f(q\hat{n}, q\hat{n}') = f^*(q\hat{n}', q\hat{n})$, see (3.2.2), and thus $|f(q\hat{n}, q\hat{n}')|^2 = |f(q\hat{n}', q\hat{n})|^2$, we encounter the situation of a product of a function that is odd in $(\hat{n}, \hat{n}')$ namely $(\hat{n} - \hat{n}') \cdot (x - x')$ with a function that is even in $(\hat{n}, \hat{n}')$, $|f(q\hat{n}, q\hat{n}')|^2$. When integrated over all directions in $\hat{n}$ and $\hat{n}'$ of q and q', the contributions to the integral due to this product term therefore average out to zero.

This leaves the expression for $F(x - x')$ in the limit $\frac{q_0 \Delta x}{\hbar} \ll 1$ as

$$F(x - x') = \int dq \varrho(q) \upsilon(q) q^2 \int \frac{d\hat{n} d\hat{n}'}{8\pi\hbar^2} \{(\hat{n} - \hat{n}') \cdot (x - x')\}^2 |f(q\hat{n}, q\hat{n}')|^2 \tag{3.3.2}$$

We now further simplify this equation, we implement the physically justifiable restriction that the scattering process is unaffected by the orientation of the scattering centre. Firstly as a consequence of this assumption we can average the term $\{(\hat{n} - \hat{n}') \cdot (x - x')\}^2$ over the possible directions $(\hat{n} - \hat{n'})$. This average is given by

$$(x - x')^2 \frac{1}{3} \sum_{i = x, y, z} \{(\hat{n} - \hat{n}') \cdot \hat{i}\}^2 = \frac{1}{3} (x - x')^2 (\hat{n} - \hat{n}')^2$$

$$= \frac{2}{3} (x - x')^2 (1 - \hat{n} \cdot \hat{n}')$$

$$= \frac{2}{3} (x - x')^2 (1 - \cos(\theta)) \tag{3.3.3}$$

here we have used θ to represent the scattering angle, by which we mean the angle between the incoming and outgoing trajectory of the scattered particles. Inserting this back into our equation,

$$F(x - x') = (x - x')^2 \int dq \varrho(q) \upsilon(q) \frac{2q^2}{3\hbar^2} \int \frac{d\hat{n} d\hat{n}'}{8\pi} (1 - \cos(\theta)) |f(q\hat{n}, q\hat{n}')|^2 \tag{3.3.4}$$

Following this we consider the cross-section $|f(q\hat{n}, q\hat{n}')|^2$ to be isotropic, meaning it only depends on the magnitude q of the momentum and the scattering angle θ. Allowing us to simplify through carrying out some of the angular integrations which yield

$$F(x - x') = (x - x')^2 \int dq \varrho(q) \upsilon(q) \frac{2\pi q^2}{3\hbar^2} \int d\cos(\theta)(1 - \cos(\theta)) |f(q, \cos(\theta))|^2 \tag{3.3.5}$$

Apart from the angular weighing term $(1 - \cos(\theta))$, the second integral can be seen as the total cross section $\sigma_{\text{tot}}(q)$ of the scattering process. Because of this we call this term the effective cross-section

$$\sigma_{\text{eff}}(q) \equiv \frac{2\pi}{3} \int d\cos(\theta)(1 - \cos(\theta)) |f(q, \cos(\theta))|^2 \tag{3.3.6}$$

which consequently is of the order of the total cross section $\sigma_{\text{tot}}(q)$.

We now step back and consider the bigger picture, particularly the time dependence of interference terms $\rho_s(x, x')$ $x \neq x'$, of the reduced density matrix of our object. Referring back to (3.2.23) and using (3.3.5) and (3.3.6), the quantitative equation for the effect of scattering on the reduced density matrix is thus,

$$\frac{\partial \rho_S(x, x', t)}{\partial t} = -\Lambda (x - x')^2 \rho_S(x, x', t) \tag{3.3.7}$$

we solve this to get,

$$\rho_S(x, x', t) = \rho_S(x, x', 0) e^{-\Lambda (\Delta x)^2 t} \tag{3.3.8}$$

where we have introduced Λ which we call (for obvious reasons) the scattering constant,

$$\Lambda \equiv \int dq \varrho(q) \upsilon(q) \frac{q^2}{\hbar^2} \sigma_{\text{eff}}(q) \tag{3.3.9}$$

From this we conclude that, in timescales short compared with the timescales for evolution of the system through the self-Hamiltonian, (3.7) shows that the scattering events lead to a suppression of off diagonal terms that increases exponentially with time and with the squared separation $(\Delta x)^2 = (x - x')^2$. Clearly the scattering constant quantifies the rate at which spatial decoherences over a given distance Δx are suppressed. From (3.3.8) we can introduce a 'decoherence timescale', (T_{Δ_x}) defined as

$$T_{\Delta_x} = \frac{1}{\Lambda (\Delta x)^2} \tag{3.3.10}$$

which is self-evidently the characteristic time required to damp spatial coherences over a distance Δx by a factor of e.

We are finally ready to obtain some numerical data which will allow us to get an idea of the decoherence timescales involved. In this next section we shall merely consider scattering of photons, but it is easy to see that with minimal changes we could obtain information about scattering of air molecules or many other environments.

3.4 Photon Scattering

We will consider a photon-gas environment at temperature T and our system as a dielectric sphere of radius a, with the assumption that we have independence between the frequency of the photon and the dielectric constant ε. By basing our work on "Long-Wavelength Limit" we guarantee upper bounds on the decoherence timescales.

If we consider the Rayleigh cross-section (where we have averaged over the different polarizations of the photons), we have

$$|f(q\hat{n}, q\hat{n}')|^2 = \left(\frac{q}{\hbar}\right)^4 a^6 \left(\frac{\varepsilon - 1}{\varepsilon + 2}\right)^2 \frac{1}{2}(1 + \cos^2(\Theta)) \tag{3.4.1}$$

Where clearly this cross-section depends on the magnitude q of the momentum and the scattering angle Θ between the directions $\hat{n}$ and $\hat{n}'$ of the particle before and after the scattering.

We continue by calculating the effective cross section $\sigma_{\text{eff}}(q)$ for the Rayleigh cross section (3.4.1). From (3.3.6) we get

$$\sigma_{\text{eff}}(q) = \left(\frac{q}{\hbar}\right)^4 a^6 \left(\frac{\varepsilon - 1}{\varepsilon + 2}\right)^2 \frac{\pi}{3} \int_{\Theta=0}^{\Theta=\pi} d\cos(\Theta)(1 - \cos(\Theta))(1 + \cos^2(\Theta))$$

$$= \frac{8\pi}{9} \left(\frac{q}{\hbar}\right)^4 a^6 \left(\frac{\varepsilon - 1}{\varepsilon + 2}\right)^2 \tag{3.4.2}$$

The scattering-constant Λ, (see (3.3.9)) requires that we obtain the momentum density $\varrho(q)$. Assuming for simplicity black-body radiation, the average occupation number of photons of energy cq at temperature T is given by the Planck distribution

$$\langle n(q)\rangle_T = \frac{2}{e^{cq/k_B T} - 1} \tag{3.4.3}$$

c being the speed of light, the factor 2 resulting from the two directions of polarization for the photons. The number density $\varrho(q)$ is obtained by multiplying $\langle n(q)\rangle_T$ by the number of states per unit volume with momenta between q and $q + dq$, which (assuming an isotropic distribution of momenta) is given by,

$$\frac{1}{(2\pi\hbar)^3} d^3 q = \frac{1}{2\pi^2\hbar^3} q^2 dq \tag{3.4.4}$$

where the change has been made from Cartesian co-ordinates to spherical polars, as well as implementing that this amount depends only on the magnitude of q, not direction, leaving $4\pi q^2$ as a new prefactor. Meaning our number density is given by

$$\varrho(q) = \frac{1}{\pi^2\hbar^3} \left(\frac{q^2}{e^{cq/k_B T} - 1}\right) \tag{3.4.5}$$

finally allowing us to calculate the resulting scattering constant Λ, using (3.3.9)

$$\begin{aligned}
\Lambda &= \int dq \varrho(q) \upsilon(q) q^2 \sigma_{\text{eff}}(q) \\
&= \int dq \frac{1}{\pi^2\hbar^3} \left(\frac{q^2}{e^{cq/k_B T} - 1}\right) c \frac{q^2}{\hbar^2} \frac{8\pi}{9} \left(\frac{q}{\hbar}\right)^4 a^6 \left(\frac{\varepsilon - 1}{\varepsilon + 2}\right)^2 \\
&= \frac{8}{9\pi\hbar^9} a^6 c \left(\frac{\varepsilon - 1}{\varepsilon + 2}\right)^2 \int dq \frac{q^8}{e^{cq/k_B T} - 1}.
\end{aligned} \tag{3.4.6}$$

This final integral may be evaluated using the Riemann ζ-function for integer arguments n,

$$\zeta(n) = \frac{1}{(n-1)!} \int_0^\infty dx \frac{x^{n-1}}{e^x - 1} \tag{3.4.7}$$

when we include $x = cq/k_B T$ and $n = 9$, we finally obtain

$$\Lambda = 8! \frac{8}{9\pi} a^6 c \left(\frac{\varepsilon - 1}{\varepsilon + 2}\right)^2 \left(\frac{k_B T}{\hbar c}\right)^9 \zeta(9) \propto a^6 T^9 \tag{3.4.8}$$

where $\zeta(9) \approx 1.002$. It's clear how strongly Λ depends on the size a and the temperature T. For example increasing T by a factor of two makes the decoherence rate more than 500 times larger.

Expanding constants in (4.8), and assuming $\left(\frac{\varepsilon - 1}{\varepsilon + 2}\right) \approx 1$, yields the scattering rate

$$\Lambda \approx 10^{20} \frac{1}{\text{cm}^2 s} \left(\frac{a}{\text{cm}}\right)^6 \left(\frac{T}{K}\right)^9 \tag{3.4.9}$$

Let us use this expression to compute a couple of numerical estimates for Λ. Consider photons at approximately $T = 300K$ (room temperature) and an object of size $a = 10^{-4}$ cm, we obtain $\Lambda \approx 10^{18} \text{cm}^{-2} s^{-1}$. Using (3.3.8) this means that spatial interferences over distances on the order of as little as $\Delta x = |x - x'| \approx 10^{-9}$ cm will become effectively suppressed within the time span of a second. Separations on the order of the size of the object ($\Delta x \approx 10^{-4}$ cm) will become significantly damped within a mere 10^{-10} seconds. If we consider a similar object now in an environment of cosmic microwave background radiation (which consists of photons at the characteristic temperature 3K), resulting in a decoherence timescale increased by a factor of 10^{18}. This rate nevertheless corresponds to an efficient decoherence process, since separations on the order of 1cm will be locally suppressed by a factor e on a timescale of a second.

Let us briefly consider what such results should tell us. Firstly, we see that decoherence is very efficient at suppressing superpositions even in an environment comprisiong only photons. This should immediately indicate the solution to one of our earlier problems which we termed the 'problem of Non-Interference', since it is clear that decoherence prevents observations of superpositions under any 'normal' conditions. Secondly, these results should tell us that any assumptions from now on that $\tau_{\text{deco}} \gg \tau_{\text{evol}}$, should be easily justified provided we have an environment at any temperature sufficiently high. We finally note that, as expected, decoherence naturally occured in the position basis as a result of other assumptions about the nature of the interaction. We now summarise the main steps in this derivation.

3.5 Summary

- Consider first scattering event by scattering matrix $\hat{S}$,

$$|x\rangle|\phi_i\rangle \longrightarrow \hat{S}|x\rangle|\phi_i\rangle$$

With the assumption that the scattering interaction is invariant under spatial translations of the joint system-environment, and the more limiting assumption that scattering has a negligible effect on our system of interest

$$|x\rangle \hat{S}|\phi_i\rangle = |x\rangle|\phi(x)\rangle$$

where the subscript x denotes that the scattering occurs at x.

- Changing to density operator notation,

$$\hat{\rho}(0) = \int dx \int dx' \rho_S(x, x', 0)|x\rangle\langle x'| \otimes |\phi_i\rangle\langle\phi_i|$$

then evolves to

$$\hat{\rho} = \int dx \int dx' \rho_S(x, x', 0)|x\rangle\langle x'| \otimes |\phi(x)\rangle\langle\phi(x')|$$

which, when we trace over the environment, using the trace function introduced in the previous chapter we obtain

$$\hat{\rho}_S = Tr_\varepsilon\hat{\rho} = \rho_S(x, x', 0)|x\rangle\langle x'| \otimes \langle\phi(x')|\phi(x)\rangle$$

- We thus consider from here, the overlap $\langle\phi(x)|\phi(x')\rangle = \langle\phi_i|\hat{S}_x\hat{S}_x^\dagger|\phi_i\rangle$ which encapsulates the act of decoherence as it is this value that effects the interference terms

- A change of basis from $\hat{S}$ into a conveniently defined function $\hat{T}$ (which is diagonal in the momentum basis $|q\rangle$), imposing a box normalisation condition and using that $\hat{S}$ is unitary gives,

$$\langle\phi(x')|\phi(x)\rangle = \frac{(2\pi\hbar)^3}{V} \sum_{q\epsilon Q_V} \mu(q) \left\{ \hat{I} - \sum_{q\epsilon Q_V}(1 - e^{i(q-q')\cdot(x-x')/\hbar})|\langle q|\hat{T}|q'\rangle|^2 \right\}$$

where $\mu(q)$ is the momentum-space density, Q_V is the set of all $q = \tilde{q}$ which fulfill periodic boundary conditions in V and q' is the eigenvalue of $\hat{T}|\tilde{q}\rangle$.

- Introducing a time-parameter T to denote time-elapsed in the scattering process. We have here made the implicit assumption that the timescale of the self-Hamiltonian of the system is much greater than the decoherence timescale.

- By using the assumption that the density of incoming particles is isotropic and taking the differential limit we find

$$\frac{\partial\rho_S(x, x', t)}{\partial t} = -F(x - x')\rho_S(x, x', t)$$

where

$$F(x - x') = \int dq\rho(q)v(q) \int \frac{d\hat{n}d\hat{n}'}{4\pi}(1 - e^{i(q-q')\cdot(x-x')/\hbar})|f(q\hat{n}, q\hat{n}')|^2$$

with $\rho(q)$ being the density of incoming particles and $v(q)$ the velocity of particles.

- We restricted ourselves to the Long-Wavelength Limit by which we mean where the wavelength λ_0 is much longer than the coherent separation. This means that it takes many scattering interactions to cause wavefunction collapse and as such is an upper bound on our decoherence timescale.

- We expand $e^{i(q-q')\cdot(x-x')/\hbar}$ up to second order and ignore higher order terms since the Long-wavelength assumptions is equivalent to $\frac{q_0\Delta(x)}{\hbar} \ll 1$.

- We make the assumption that the orientation of time scattering centre does not effect the scattering process, and thus average the term $\{(\hat{n} - \hat{n}') \cdot (x - x')\}^2$ over the possible directions $(\hat{n} - \hat{n}')$.

- We consider the cross-section to be isotropic i.e., $|f(q\hat{n}, q\hat{n}')|^2$ depends only on the magnitude of q and the scattering angle θ. Inserting this we get,

$$F(x - x') = (x - x')^2 \int dq\rho(q)v(q)\frac{2\pi q^2}{3\hbar^2} \int d\cos(\theta)(1 - \cos(\theta))|f(q, \cos(\theta))|^2$$

- Defining the effective cross-section as $\sigma_{\text{eff}}(q) \equiv \frac{2\pi}{3} \int d\cos(\theta)(1 - \cos(\theta))|f(q, \cos(\theta))|^2$ we have the result

$$\rho_S(x, x', t) = \rho_S(x, x', 0)e^{-\Lambda(\Delta(x))^2 t}$$

$$\Lambda \equiv \int dq\rho(q)v(q)\frac{q^2}{\hbar^2}\sigma_{\text{eff}}(q)$$

- We finally define the characteristic decoherence timescale as the time it takes for spatial coherences over a distance $\Delta(x)$ to be damped by a factor e^1, which is clearly

$$T_{\Delta_x} = \frac{1}{\Lambda(\Delta(x))^2}$$

- For a model where the system was interacting with an environment of photon-gas we used the Rayleigh cross-section and assumed blackbody radiation for the number of photons with energy cq at temperature T, as well as assuming an isotropic distribution of momenta.

- We derived the scattering constant as,

$$\Lambda = 8! \frac{8}{9\pi} a^6 c \left(\frac{\varepsilon - 1}{\varepsilon + 2}\right)^2 \left(\frac{k_B T}{\hbar c}\right)^9 \zeta(9) \propto a^6 T^9$$

where a is the size of the scattering object, T is temperature and ε is the dielectric constant.

4 Master-Equations and Canonical Models

Given the work up until this point, we have so far achieved a rather inefficient method for modelling the effect of interaction between system and environment as opposed to a closed system. By 'inefficient' we refer to the fact that each time we encounter a modified or brand new example we are effectively reduced to starting from scratch, determine the dynamics of the system-environment composite before tracing out the environmental degrees of freedom. In this chapter we will introduce two tools for simplifying this process, in order that analysis of more complex systems will become feasible and practical. We first note a couple of motivating factors that we will subsequently bear in mind, which lead us to the introduction of so-called 'Master-Equations'.

1. We generally are ultimately not interested in the dynamics of either the environment or indeed the system-environment composite, only the system.

2. Often it is extremely difficult if not impossible to analytically determine the time evolution of the density matrix, as such we implement approximations.

Given this we introduce master-equations, however this still leaves us thousands of slightly different systems being dealt with separately. This motivates the introduction of 'Canonical Models' in the second part of this chapter. Such models are very general and many other models can be mapped to one of these models, more will be said on this once we reach it.

4.1 Master-Equations Formalism

In our earlier "ordinary" formalism of decoherence, the method we used to compute the reduced density matrix $\hat{\varrho}_s(t)$ was

$$\hat{\varrho}_s(t) = \text{Tr}_\varepsilon \left\{ \hat{\varrho}_{s\varepsilon}(t) \right\} = \text{Tr} \left\{ \hat{U}(t) \hat{\varrho}_{s\varepsilon}(0) \hat{U}^\dagger(t) \right\} \tag{4.1.1}$$

where we have denoted the time-evolution operator for the system-environment composite as $\hat{U}(t)$. As noted in the introduction, such a method is cumbersome and necessitates us initially determining the dynamics of $\hat{\varrho}_{s\varepsilon}(t)$ prior to tracing over the environment and obtaining the reduced density matrix $\hat{\varrho}_s(t)$. There is no prima facie reason why this should be possible let alone easy to accomplish, indeed in some cases it is impossible to analytically to solve such dynamics.

In the master-equation formalism we instead calculate $\hat{\varrho}_s(t)$ with reference only to $\hat{\varrho}_S(0)$ using the formula

$$\hat{\varrho}_s(t) = \hat{V}(t) \hat{\varrho}_s(0) \tag{4.1.2}$$

where $\hat{V}(t)$ is called the 'dynamical map' which generates the evolution of $\hat{\varrho}_s(t)$. $\hat{V}(t)$ is an operator which acts on another operator and as such is often called a 'superoperator'. The above equation is called a 'master-equation' in its most general form. Clearly were our master-equation to be exact then such an equation would be merely a trivial rewriting of our earlier equation such that

$$\hat{V}(t) \hat{\varrho}_s(t) = \text{Tr} \left\{ \hat{U}(t) \hat{\varrho}_{s\varepsilon} \hat{U}^\dagger(t) \right\} \tag{4.1.3}$$

As such the power of master-equations results from approximations we use to determine the approximate time evolution of $\hat{\varrho}_s(t)$.

We will consider only master equations which can be written in the form

$$\frac{d}{dt} \hat{\varrho}_s(t) = \hat{\mathcal{L}} \left[\hat{\varrho}_s(t) \right] = -i \left[\hat{H}'_S, \hat{\varrho}_s(t) \right] + \hat{D} \left[\hat{\varrho}_s(t) \right] \tag{4.1.4}$$

i.e. as a first-order differential equation. Such an equation will be local in time, in the sense that changes of ϱ_s at time t do not depend on any time $t' \neq t$. The superoperator $\hat{\mathcal{L}}$, which will typically depend on the initial state as well as the Hamiltonian, has been decomposed into two terms:

1. A non-unitary part which we denoted $\hat{D} \left[\hat{\varrho}_s(t) \right]$ which represents processes such as decoherence and dissipation. As such this term will be the one we subsequently concentrate most on.

2. The term given by the standard Liouville-von Neumann commutator is the unitary contribution to the evolution. We briefly make the important observation that due to the presence of the environment $\hat{H}'_s$ is almost certainly not equivalent to the standard Hamiltonian for a free system $\hat{H}_s$. This is because the introduction of an environment often has the effect of perturbing the free Hamiltonian possibly renormalizing the energy levels of the system (Lamb-shift).

It is immediately clear that in the case of entirely unitary evolution we are left with

$$\frac{d}{dt} \hat{\varrho}_s(t) = -i \left[\hat{H}'_s, \hat{\varrho}_s(t) \right] \tag{4.1.5}$$

which differs from the case of a closed system only in the use of the environment-perturbed system Hamiltonian $\hat{H}'_s$. Having noted this, we will now attempt to find a general expression for $\hat{\mathcal{L}}$, implementing 'reasonable' assumptions along the way. Applying this to a given model should allow us to approximately determine the dynamical evolution of $\hat{\varrho}_s(t)$ for all t.

4.2 The Born-Markov Equation

We introduce two approximations that will form the basis for our following work, where the formal representation and physical requirements for these approximations will be discussed in greater depth later.

1. The Markov Approximation: This approximation roughly states that all self-correlations which form within the environment as a result of its coupling to the system decay over a characteristic timescale much shorter than the timescale of significant change to the system.

2. The Born Approximation: If we assume that the environment is 'large' and interacts with the system sufficiently weakly then changes in the environment density operator can be assumed negligible, and the system-environment density operator remains approximately separable,

$$\hat{\varrho}_{s\varepsilon}(t) \approx \hat{\varrho}_s(t) \otimes \hat{\varrho}_\varepsilon \tag{4.2.1}$$

where $\hat{\varrho}_\varepsilon$ is constant with respect to time.

It is immediately worth pointing out that in particular circumstances such as low temperatures or solid-state systems, the above approximations are not applicable due to the non-Markovian nature of the dynamics.

Let us now develop the Born-markov master-equation, where the working we shall follow mirrors that of Ch.4.2.2 of [26]. If we initially decompose the total Hamiltonian into three parts as follows,

$$\hat{H} = \hat{H}_s + \hat{H}_\varepsilon + \hat{H}_{\text{int}} \tag{4.2.2}$$

where $\hat{H}_s$ and $\hat{H}_\varepsilon$ refer to the self-Hamiltonians of the system and environment respectively and $\hat{H}_{\text{int}}$ denotes the interaction terms. Since we intend to implement perturbation theory, we switch to the so-called 'Interaction picture' [2]. As such we define

$$\hat{H}_0 = \hat{H}_s + \hat{H}_\varepsilon \tag{4.2.3}$$

which naturally is the entire free-Hamiltonian, leaving $\hat{H}_{\text{int}}$ as the part we treat perturbatively. We next put both $\hat{H}_{\text{int}}$ and $\hat{\varrho}(t)$ into the interaction picture, by which we mean

$$\hat{H}_{\text{int}}(t) = e^{i\hat{H}_0 t} \hat{H}_{\text{int}} e^{-i\hat{H}_0 t} \tag{4.2.4}$$

$$\begin{aligned}
\hat{\varrho}_{\text{int}}(t) = \hat{\varrho}^{(I)}(t) &= e^{i\hat{H}_0 t} \hat{\varrho}(t) e^{-i\hat{H}_0 t} \\
&= e^{i\hat{H}_0 t} e^{-i\hat{H}t} \hat{\varrho} e^{i\hat{H}t} e^{-i\hat{H}_0(t)}
\end{aligned} \tag{4.2.5}$$

Since we know that in the Schrödinger picture

$$\frac{d}{dt}\hat{\varrho}(t) = -i\left[\hat{H}, \hat{\varrho}(t)\right] \tag{4.2.6}$$

with $\hat{H}$ being the full Hamiltonian. We can thus, in the interaction picture, write

$$\begin{aligned}
\frac{d}{dt}\hat{\varrho}^{(I)}(t) &= i\left[\hat{H}_0(t), \hat{\varrho}^{(I)}(t)\right] + e^{i\hat{H}_0(t)}\left(\frac{d}{dt}\hat{\varrho}(t)\right)e^{-i\hat{H}(t)} \\
&= i\left[\hat{H}_0(t), \hat{\varrho}^{(I)}(t)\right] - ie^{i\hat{H}_0(t)}\left[\hat{H}(t), \hat{\varrho}(t)\right]e^{-i\hat{H}_0(t)}
\end{aligned} \tag{4.2.7}$$

We now decompose $\hat{H}(t)$ into the free and interacting parts and use linearity of the commutator to obtain,

$$\begin{aligned}
\frac{d}{dt}\hat{\varrho}^{(I)}(t) &= i\left[\hat{H}_0(t), \hat{\varrho}^{(I)}(t)\right] - ie^{i\hat{H}_0(t)}\left[\hat{H}_0(t) + \hat{H}_{\text{int}}, \hat{\varrho}(t)\right]e^{-i\hat{H}_0(t)} \\
&= -ie^{i\hat{H}_0(t)}\left[\hat{H}_{\text{int}}, \hat{\varrho}(t)\right]e^{-i\hat{H}_0(t)}
\end{aligned} \tag{4.2.8}$$

which gives us the result that the evolution of the interaction-picture density operator can be expressed as a Liouville-von Neumann commutator with reference only to the interaction part of the Hamiltonian $\hat{H}_{\text{int}}$. As such we define the Liouville-von Neumann equation in the interaction picture to be

$$\frac{d}{dt}\hat{\varrho}^{(I)}(t) = -i\left[\hat{H}_{\text{int}}(t), \hat{\varrho}^{(I)}(t)\right] \tag{4.2.9}$$

We now proceed to integrate (4.2.9), which gives us

$$\hat{\varrho}^{(I)}(t) = \hat{\varrho}(0) - i\int_0^t dt'\left[\hat{H}_{\text{int}}(t'), \hat{\varrho}^{(I)}(t')\right] \tag{4.2.10}$$

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[2]The Interaction picture (or Dirac picture) is intermediate between the Schrödinger and Heisenberg pictures, in that rather than only one of either the state vector or operators carrying the time dependence, both carry part of the time-dependence. See Appendix of [26].

taking this expression for $\hat{\varrho}^{(I)}(t)$ we use it on the right-hand side of equation (4.2.9) obtaining

$$\frac{d}{dt}\hat{\varrho}^{(I)}(t) = -i\left[\hat{H}_{\text{int}}(t), \hat{\varrho}(0) - i\int_0^t dt' \left[\hat{H}_{\text{int}}(t'), \hat{\varrho}^{(I)}(t')\right]\right]$$

$$= -i\left[\hat{H}_{\text{int}}, \hat{\varrho}(0)\right] - \int_0^t dt' \left[\hat{H}_{\text{int}}(t)\left[\hat{H}_{\text{int}}(t'), \hat{\varrho}^{(I)}(t)\right]\right] \tag{4.2.11}$$

We trace over the environment, much as before, thus giving us an equation for the reduced density operator $\hat{\varrho}_s^{(I)}(t)$, namely

$$\frac{d}{dt}\hat{\varrho}_s^{(I)}(t) = -i\text{Tr}_\varepsilon\left[\hat{H}_{\text{int}}(t), \hat{\varrho}(0)\right] - \int_0^t dt' \text{Tr}_\varepsilon\left[\hat{H}_{\text{int}}(t)\left[\hat{H}_{\text{int}}(t'), \hat{\varrho}^{(I)}(t)\right]\right] \tag{4.2.12}$$

Without loss of generality we set

$$\text{Tr}_\varepsilon\left[\hat{H}_{\text{int}}, \hat{\varrho}(0)\right] = 0 \tag{4.2.13}$$

which can simply be achieved through a formal redefinition of our Hamiltonians $\hat{H}_0$ and $\hat{H}_{\text{int}}$. As such we simplify equation (4.2.12) to

$$\frac{d}{dt}\hat{\varrho}_s^{(I)}(t) = -\int_0^t \text{Tr}_\varepsilon\left[\hat{H}_{\text{int}}(t), \left[\hat{H}_{\text{int}}(t'), \hat{\varrho}^{(I)}(t')\right]\right] dt' \tag{4.2.14}$$

Where upto this point we have been exact in our calculations, we now resort to approximations. We begin by considering which properties we desire for a master-equation which are currently absent from equation (4.2.14).

Most notably, when we initially introduced master-equations we stipulated that such an equation would be time-local which, since equation (4.2.14) depends on all times 0 to t, we clearly do not yet satisfy. As such two desirable properties emerge;

- Firstly, we wish to remove all dependence in the change of $\hat{\varrho}_s^{(I)}(t)$ at times $t' < t$. An equation which depends on times preceding the moment of change is known as an integro-differential equation.

- Secondly, we wish to obtain our original goal and describe the evolution purely in terms of $\hat{\varrho}_s(t)$ and $\hat{\varrho}_\varepsilon(0)$.

We accomplish these aims by using the approximations mentioned earlier, namely the Markov and Born approximations. Initially we impose the Born approximation allowing us to eliminate our dependence on $\hat{\varrho}_\varepsilon(t)$ leaving an integro-differential equation and dealing with our second requirement. Following this we use the Markov approximation to give us a time-local differential equation and thus satisfying our first requirement. As we discuss below, implementation of such justifications is motivated by weak interaction between the system and the environment as well as an environment much larger than the system. Before we impose these approximations we make one further remark, namely we make the standard assumption that at $t = 0$ there are no existing correlations between the system and the environment, i.e.

$$\hat{\varrho}(0) = \hat{\varrho}_s(0) \otimes \hat{\varrho}_\varepsilon(0) \tag{4.2.15}$$

Certainly in the case of weak system-environment interaction such an assumption is reasonable.

We start by implementing the Born approximation, where we assume that the density operator remains at all times approximately separable and that temporal variation in the environmental density matrix may be neglected, so that

$$\hat{\varrho}(t) \approx \hat{\varrho}_s(t) \otimes \hat{\varrho}_\varepsilon(0) \tag{4.2.16}$$

since $\hat{\varrho}^{(I)}(t) = e^{i\hat{H}_0 t}\hat{\varrho}(t)e^{-i\hat{H}_0 t}$, with $\hat{H}_0 = \hat{H}_s + \hat{H}_\varepsilon$, it is clear that $\hat{H}_s$ and $\hat{H}_\varepsilon$ act separately on the system and environment respectively. As a result of this it is clear that no entanglement can be established as a result and we can write an analogous result to (4.2.16) in the interaction picture,

$$\hat{\varrho}^{(I)}(t) \approx \hat{\varrho}_s^{(I)}(t) \otimes \hat{\varrho}_\varepsilon(0) \tag{4.2.17}$$

$\forall t \geq 0$.

The reasoning behind the Born approximation is that; in the "weak-coupling limit" and for a suitably large environment compared to the system, then (i) the system and environment remain approximately separable at all times and (ii) the environmental density operator remains effectively unchanged as a result of the interaction. It turns out that in many physical systems of interest the Born approximation is entirely legitimate. The system is often coupled to a comparably large environment which undergoes negligibly small alterations as a result of the interaction as compared to the system. Note that (4.2.17) still permits arbitrary large changes to $\hat{\varrho}_s^{(I)}(t)$ and it does not exclude the occurrence in the environment of excitations induced by interaction with the system.

Once we use the Born approximation (4.2.17) on our master-equation (4.2.14), we obtain an equation of the form

$$\frac{d}{dt}\hat{\varrho}_s^{(I)}(t) = -\int_0^t dt' \text{Tr}_\varepsilon\left[\hat{H}_{\text{int}}(t), \left[\hat{H}_{\text{int}}(t'), \hat{\varrho}_s^{(I)}(t') \otimes \hat{\varrho}_\varepsilon(0)\right]\right] \tag{4.2.18}$$

35

where we have evidently expressed our master-equation entirely in terms of $\hat{\varrho}_s^{(I)}(t)$ and $\hat{\varrho}_\varepsilon(0)$ and thus satisfied our second requirement. However, as mentioned previously, equation (4.2.18) is still an integro-differential equation that is, to compute the change of $\hat{\varrho}_s^{(I)}(t)$ at time t correctly, requires that we are aware of the behaviour for previous times $t' < t$. In order that we may rectify this situation (by use of the Markov approximation), let us write the interaction Hamiltonian in the diagonal form

$$\hat{H}_{\text{int}} = \sum_\alpha \hat{S}_\alpha(t) \otimes \hat{E}_\alpha \tag{4.2.19}$$

and transform this into the interaction picture,

$$\begin{aligned}
\hat{H}_{\text{int}}(t) &= e^{i\hat{H}_0 t} \hat{H}_{\text{int}} e^{-i\hat{H}_0 t} \\
&= \sum_\alpha \left(e^{i\hat{H}_0 t} \hat{S}_\alpha e^{-i\hat{H}_0 t} \right) \left(e^{i\hat{H}_0 t} \hat{E}_\alpha e^{-i\hat{H}_0 t} \right) = \sum_\alpha \hat{S}_\alpha \otimes \hat{E}_\alpha(t)
\end{aligned} \tag{4.2.20}$$

which allows us to express our equation (4.2.18) in the form

$$\frac{d}{dt}\hat{\varrho}_s(t) = -\int_0^t dt' \sum_{\alpha\beta} \text{Tr}_\varepsilon \left[\hat{S}_\alpha(t) \otimes \hat{E}_\alpha(t), \left[\hat{S}_\beta(t') \otimes \hat{E}_\beta(t'), \hat{\varrho}_s^{(I)}(t') \otimes \hat{\varrho}_\varepsilon(0) \right] \right] \tag{4.2.21}$$

We continue from here by making the definition

$$C_{\alpha\beta}(t,t') := \text{Tr}_\varepsilon \left\{ \hat{E}_\alpha(t) \hat{E}_\beta(t') \hat{\varrho}_\varepsilon \right\} \tag{4.2.22}$$

We shall now make the further assumption that the environment is in equilibrium, such that it remains in a single state. As such $\left[\hat{H}_\varepsilon, \hat{\varrho}_\varepsilon \right] = 0$ and we may thus write

$$C_{\alpha\beta}(t,t') = \text{Tr}_\varepsilon \left\{ E_\alpha(t-t') \hat{E}_\beta \hat{\varrho}_\varepsilon \right\} \equiv C_{\alpha\beta}(t-t') \tag{4.2.23}$$

which we call the environmental self-correlation functions. The reasoning behind this terminology is simple: the operators $\hat{E}_\alpha$ can be thought of as "observables" measured on the system (provided they are Hermitian). The environment self-correlation function tells us in what manner the result of such a measurement effects the same measurement carried out at a time $t - t'$ later. Thus loosely speaking this function quantifies the extent to which the environment retains information regarding its interaction with our system over time. Introducing these into our equation (4.2.18) having expanded out the commutators we find

$$\begin{aligned}
\frac{d}{dt}\hat{\varrho}_s^{(I)}(t) = -\text{Tr}_\varepsilon \int_0^t dt' \sum_{\alpha\beta} &\left\{ \hat{S}_\alpha(t) \hat{E}_\alpha(t) \hat{S}_\beta(t') \hat{E}_\beta(t') \hat{\varrho}_s^{(I)}(t') \hat{\varrho}_\varepsilon(0) - \hat{S}_\alpha(t) \hat{E}_\alpha(t) \hat{\varrho}_s^{(I)}(t') \hat{\varrho}_\varepsilon(0) \hat{S}_\beta(t') \hat{E}_\beta(t') \right\} \\
&- \left\{ \hat{S}_\beta(t') \hat{E}_\beta(t') \hat{\varrho}_s^{(I)}(t') \hat{\varrho}_\varepsilon(0) \hat{S}_\alpha(t) \hat{E}_\alpha(t) - \hat{\varrho}_s^{(I)}(t') \hat{\varrho}_\varepsilon(0) \hat{S}_\beta(t') \hat{E}_\beta(t') \hat{S}_\alpha(t) \hat{E}_\alpha(t) \right\}
\end{aligned} \tag{4.2.24}$$

and since the trace operation is invariant under cyclic permutations we may further rewrite this into the more compact form

$$\begin{aligned}
\frac{d}{dt}\hat{\varrho}_s^{(I)}(t) = -\int_0^t dt' \sum_{\alpha\beta} &\left\{ C_{\alpha\beta}(t-t') \left[\hat{S}_\alpha(t) \hat{S}_\beta(t') \hat{\varrho}_s^{(I)}(t') - \hat{S}_\beta(t') \hat{\varrho}_s^{(I)}(t') \hat{S}_\alpha(t) \right] \right\} \\
&+ \left\{ C_{\beta\alpha}(t'-t) \left[\hat{\varrho}_s^{(I)}(t') \hat{S}_\beta(t') \hat{S}_\alpha(t) - \hat{S}_\alpha(t) \hat{\varrho}_s^{(I)}(t') \hat{S}_\beta(t') \right] \right\}
\end{aligned} \tag{4.2.25}$$

We have also here separated out the $\hat{S}_\alpha$ and $\hat{S}_\beta$ operators as well as the density matrix $\hat{\varrho}_s^{(I)}(t)$ from the trace operation, which is clearly legitimate since the trace here only refers to the environment.

It is at this point that we implement our second approximation, namely the Markov approximation. In many situations of interest, the environment can be assumed to quickly 'forget' self-correlations. That is, in such cases where the environment doesn't "keep track of it's history" - dynamically established quantum correlations within the environment decay on a timescale τ_{corr} much shorter than the timescale τ_s set by the evolution of $\hat{\varrho}_s(t)$ to change 'noticeably'. Such an approximation $(\tau_{\text{corr}} \ll \tau_s)$ is entirely reasonable provided that the environment is of a sufficiently high temperature as well as being weakly coupled to the system. The result of such an approximation to our master-equation is that the environmental self-correlation functions are dominated by the values near $(t - t') = 0$, decaying on a timescale much shorter than that set by $\hat{\varrho}_s^{(I)}(t')$. This has two implications for our master-equation: firstly, since $\hat{\varrho}_s^{(I)}(t)$ changes insignificantly over times where $C_{\alpha\beta}$ is non-negligible, we replace the retarded-time density operator $\hat{\varrho}_s^{(I)}(t')$ by the current-time density operator $\hat{\varrho}_s^{(I)}(t)$ in the right-hand side of (4.2.25). The resulting master equation is the so-called Redfield equation and satisfies all our desired properties. However, the Markov assumption allows us one final simplification: we note that for $t \gg \tau_{\text{corr}}$ the lower limit of

integration can be extended to $-\infty$ since the self-correlation functions $C_{\alpha\beta}(t-t^{'})$ suppress the integrand for $t^{'} \ll t$. This finally allows us to write the Born-Markov master-equation in the interaction picture as

$$\frac{d}{dt}\hat{\varrho}_s^{(I)}(t) = -\int_0^\infty d\tau \sum_{\alpha\beta} C_{\alpha\beta}(\tau)\left[\hat{S}_\alpha(t)\hat{S}_\beta(t-\tau)\hat{\varrho}_s^{(I)}(t) - \hat{S}_\beta(t-\tau)\hat{\varrho}_s^{(I)}(t)\hat{S}_\alpha(t)\right]$$
$$+ C_{\beta\alpha}(-\tau)\left[\hat{\varrho}_S^{(I)}(t)\hat{S}_\beta(t-\tau)\hat{S}_\alpha(t) - \hat{S}_\alpha(t)\hat{\varrho}_s^{(I)}(t)\hat{S}_\beta(t-\tau)\right] \tag{4.2.26}$$

where $\tau = t - t^{'}$ now goes between ∞ and 0 which we have swapped by taking a minus sign outside the integral. As we required, the right-hand side no longer requires knowledge of the full time-dependent density operator $\hat{\varrho}^{(I)}(t)$, merely the reduced density operator, local in time $\hat{\varrho}_s^{(I)}(t)$ along with the initial state of the environment. As such, only completely known quantities $\hat{S}_\alpha(t)$ and $\hat{E}_\alpha(t)$ (which are determined by the form of the Hamiltonian) are present in equation (4.2.26) with arguments which differ from the 'current-time' t.

Equation (4.2.26) is essentially our key result, we now simply rewrite our result into the Schrödinger picture. Recall from earlier that

$$\frac{d}{dt}\hat{\varrho}_s(t) = -i\left[\hat{H}_s, \hat{\varrho}_s(t)\right] + e^{-i\hat{H}_s t}\left(\frac{d}{dt}\hat{\varrho}_s^{(I)}(t)\right)e^{i\hat{H}_s t} \tag{4.2.27}$$

Applying this reasoning, for example, to the first term in square brackets, we find

$$e^{-i\hat{H}_s t}\hat{S}_\alpha(t)\hat{S}_\beta(t-\tau)\hat{\varrho}_s^{(I)}(t)e^{i\hat{H}_s t} = \left(e^{-i\hat{H}_s t}\hat{S}_\alpha(t)e^{i\hat{H}_s t}\right)\left(e^{-i\hat{H}_s t}\hat{S}_\beta(t-\tau)e^{i\hat{H}_s t}\right)\left(e^{-i\hat{H}_s t}\hat{\varrho}_s^{(I)}(t)e^{i\hat{H}_s t}\right)$$
$$= \hat{S}_\alpha\hat{S}_\beta(-\tau)\hat{\varrho}_s \tag{4.2.28}$$

In this way we rewrite (4.2.26) into the form

$$\frac{d}{dt}\hat{\varrho}_s(t) = -i\left[\hat{H}_s, \hat{\varrho}_s(t)\right] - \int_0^\infty d\tau \left\{C_{\alpha\beta}(\tau)\left[\hat{S}_\alpha, \hat{S}_\beta(-\tau)\hat{\varrho}_s(t)\right] + C_{\beta\alpha}(-\tau)\left[\hat{\varrho}_s(t)\hat{S}_\beta(-\tau), \hat{S}_\alpha\right]\right\} \tag{4.2.29}$$

where we have reintroduced the commutators. We make a final simplification by realizing that the integral on the right-hand side effectively integrates out all time dependence on $C_{\alpha\beta}(\tau)$ and $\hat{S}_\beta(\tau)$. Thus we define the time-independent quantities $\hat{B}_\alpha$ and $\hat{C}_\alpha$ as,

$$\hat{B}_\alpha := \int_0^\infty d\tau \sum_\beta C_{\alpha\beta}(-\tau)\hat{S}_\beta(-\tau)$$
$$\hat{C}_\alpha := \int_0^\infty d\tau \sum_\beta C_{\beta\alpha}(-\tau)\hat{S}_\beta(-\tau) \tag{4.2.30}$$

which, when substituted, leaves the final form for the Born-Markov master-equation, namely

$$\frac{d}{dt}\hat{\varrho}_s(t) = -i\left[\hat{H}_s, \hat{\varrho}_s(t)\right] - \sum_\alpha \left\{\left[\hat{S}_\alpha, \hat{B}_\alpha\hat{\varrho}_s(t)\right] + \left[\hat{\varrho}_s(t)\hat{C}_\alpha, \hat{S}_\alpha\right]\right\} \tag{4.2.31}$$

We shall return to this later in the chapter in order that we may illustrate the application of such an equation to a canonical model (the so-called 'Spin-Boson model'). However, before this we introduce the topic of Canonical Models.

4.3 Canonical Models

As referred to earlier, as it stands each time we encounter a fresh example we must start from scratch in developing a model. Even the introduction of master-equations has not reduced the sheer volume of possible systems, it has merely made the calculation of a given model easier under certain conditions. So it is natural to ask whether there exists a smaller set of models onto which we could 'map' a much larger amount of models. Fortunately the answer to this is yes, in such so-called 'canonical models', the central system is represented either by a two-state system (if the state-space of the system is discrete and effectively two-dimensional), or by a particle described in continuous coordinates which is subject to some form of potential (e.g. a harmonic oscillator potential). The environment is likewise modelled as a collection of spin-$\frac{1}{2}$ particles or oscillators and are thus commonly referred to as either spin-environment models or oscillator-environment models.

It is immediately obvious that this leaves us four possible combinations of systems and environments. These canonical models are extremely useful, since the details of a specific system interacting with a specific environment are encapsulated in the choice of canonical model and the subsequent parameters. As such once the model has been solved for arbitrary parameters it is comparatively easy to adapt to the intended model by subsequent choice of parameters.

Before we embark on a more detailed analysis of these models, let us first discuss the motivation behind the 'mappings' referred to above. It is certainly not obvious in what manner the vast array of possible systems and environments may be reduced to a combination of harmonic oscillators and spin-$\frac{1}{2}$ particles. It is however worth noting the parallels in that the central tenet of statistical mechanics is that dynamics of the system and more importantly the environment may be

essentially captured by only a few coordinates. In the case of the system this means that even if the underlying microscopic structure is much more complex, we may describe the system by one or two-coordinates, which may be either discrete or continuous.

Let us begin by considering a central two-state system, this most often results from the truncation of a continuous coordinate by a potential into two minimum energies separated by a potential barrier, such as the one shown in Fig.6, where we obviously require suitably low energy. As such the dynamics are those of a particle confined to a double-well potential, where, in most cases of interest, only one or two states including the ground states are present in each well and typically the excited states will not be populated. The result of all this is to yield effectively our required two-state system, where each state refers to position in the left or right well. From here we map our states onto the quantum states $|0\rangle$ being "spin-down" and $|1\rangle$ being "spin-up", of a spin-$\frac{1}{2}$ particle. Such two-level systems are particularly relevant in quantum computing, since they represent the "qubit" (quantum bit) used to encode information.
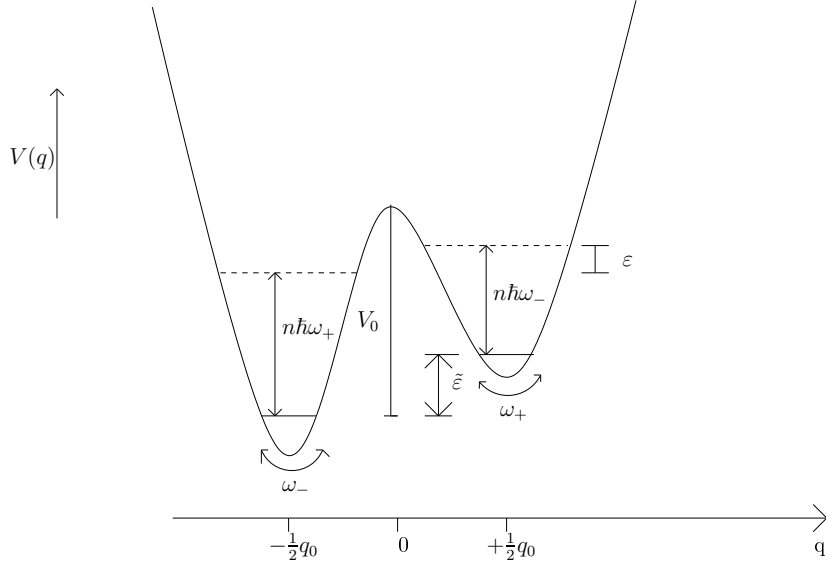

Figure 6: The truncated double-well potential, we choose the origin so that the wells are centred at $\pm\frac{q_0}{2}$ and $\tilde{\varepsilon}$ is the disparity between the ground-state energies called the "asymmetry energy".

The dynamics of the system result from quantum tunneling (which we reviewed in the first chapter), between the two wells. The energy spacings within each well are generally large compared to the gap between the two ground state energies (the "asymmetry energy"), and this ensures that the particle cannot tunnel from one well to the other and end up in a state other than the ground state in the new well.

For continuous coordinates by contrast, we typically use co-ordinates $\hat{X}$ (position) and $\hat{P}$ (momentum) describing a mass-point in phase-space which moves in some potential $V(\hat{X})$. Two cases of particular interest to quantum mechanics and studies of decoherence are those of the free-particle ($V(\hat{X}) = 0$) and harmonic oscillator ($V(\hat{X}) = M\Omega^2\frac{\hat{X}^2}{2}$). The harmonic-oscillator potential for example is often used to represent a particle confined to a "trap" for example a crystal lattice or magnetic field.

The choice of position and momentum as the relevant coordinates result from interactions with the environment, namely the environment induced superselection we discussed earlier. In many key instances, such as Quantum Brownian Motion (a harmonic oscillator linearly coupled to an environment of harmonic oscillators), the evolution of the system is governed in approximately equal strengths by the two Hamiltonians $\hat{H}_s$ and $\hat{H}_{\text{int}}$. Since the majority of interactions in nature are dependent on the separation of interacting particles, $\hat{H}_{\text{int}}$ will typically be diagonalizable in the position coordinate. In contrast, the kinetic-energy term of the self-Hamiltonian is $\frac{M\hat{P}^2}{2}$ and is thus diagonal in momentum. Therefore we typically emerge with a compromise between complete localization in position and complete localization in momentum, which leads to states approximately localized in phase-space. For an accessible analysis of the Quantum Brownian Motion model which displays these characteristics particularly clearly in the Wigner representation, see Ch.5 of [26].

If we now turn to a consideration of mapping the environment, two cases must again be considered. If we again initially consider spin environments, then we remark that this is the most applicable model when we consider low-temperature examples. By low we here refer to temperatures which are not obtained in the everyday world we encounter, but are routinely reached in the laboratory. These conditions are most notably important in experiments on quantum coherence and decoherence, such as those involving superconductors, where these experiments require temperatures very close to absolute zero. Indeed it is experiments such as these which are analysed in the hope of realizing qubit systems and in turn quantum computers. From the above discussion it is evident why stress is placed on accurately modeling decoherence in the regime of

low-temperatures. Experimental evidence indicates that in this case, decoherence primarily results from interactions between the system and localized modes such as nuclear spins, defects and paramagnetic electronic impurities. The division between this and oscillator environments results from the localization of the wave functions describing such effects, meaning that the wave function is confined to a small region in space as compared to those of the oscillators. Localized modes such as these are described by a finite-dimensional Hilbert Space and a finite energy cutoff.

Given this we model these modes using discrete states and mapping from this onto a spin-system. In the majority of interesting cases there are only two discrete states and as such we map our environment onto one which constitutes spin-$\frac{1}{2}$ particles. We now briefly distinguish between an "internal environment", where the spin-environment modes exist as part for the system of interest, and cases where the modes are part of the surrounding substrate. In superconducting-quantum-interference devices (SQUIDS), the coordinate associated to the flux couples electromagnetically to both the nuclear spins which primarily constitute the SQUID within penetration depth of the flux, as well as impurities present in the material.

The literature is inundated by examples in which spin-environments are both significant and even dominant, in the effects of decoherence, researchers are able to create mesoscopic or indeed macroscopic coherent-superpositions. This thermal environment refers to the bath of harmonic oscillators (delocalized bosonic modes) which we will discuss next. However, once we have lowered the temperature to the region of absolute zero, such as in the SQUIDs mentioned above, decoherence becomes largely due to those modes which are mostly if not entirely unaffected by the low-temperature, such as nuclear spins or impurities present within our material.

If we now turn our attention to environments which constitute oscillators, be begin by remarking that such environments represent a quasi-continuum of bosonic field modes where energy as well as coherence are lost irrevocably from the central system into the environment. These bosonic modes are also delocalized in contrast to before, meaning that the wave function for each constituent oscillator is spread out over a relatively large spatial domain. Such a delocalization in the modes of the environment is a feature which is characteristic of harmonic-oscillator environments.

Oscillator environments are extremely general and such diversity makes them very useful and as such important. It is possible to show that for energies which are sufficiently low, a whole host of interacting system-environment composites may be effectively represented by an environment of harmonic oscillators, which are linearly coupled to a system described by only one or two coordinates. This fact motivates our subsequent interest in the spin-boson model (a central two-state system linearly coupled to an oscillator-environment), indeed more formally Feynman and Vernon [23] demonstrated that when interaction between system and environment is sufficiently weak then any environment can be rigorously mapped onto a system, linearly coupled to a collection of harmonic oscillators. Such a result is clearly magnificent for our task of reducing the sheer volume of work required to model decoherence generally and it would be fantastic to follow up this work. However, it is neither short nor simple and would take us too far from our subject of interest, I therefore leave it to the reader to follow such a line of inquiry further should they wish and here we shall simply use the result. We now apply our discussion up to this point regarding both master-equations and canonical models to analyze the so-called 'spin-boson model'.

4.4   Born-Markov Master-Equation for the Spin-Boson Model

First, we decompose our Hamiltonian into three sections as before and concentrate on those parts which pertain to the environment

$$\hat{H} = \hat{H}_s + \hat{H}_\varepsilon + \hat{H}_{\text{int}} \tag{4.4.1}$$

So while we leave $\hat{H}_s$ unspecified, we consider that $\hat{H}_\varepsilon$ refers to a collection of harmonic oscillators which by assumption do not interact. Therefore $\hat{H}_\varepsilon$ is simply the sum of single-oscillator Hamiltonians given by

$$\hat{H}_\varepsilon = \sum_i \left(\frac{1}{2m} \hat{p}_i^2 + \frac{1}{2} m_i \omega_i^2 \hat{q}_i^2 \right) \tag{4.4.2}$$

where as in the standard notation m_i and ω_i refer to the mass and natural frequency of the ith oscillator respectively, and $\hat{p}_i$ and $\hat{q}_i$ denote the canonical momentum and position operators acting on the ith particle.

The interaction Hamiltonian is such that the spin coordinate $\hat{\sigma}_z$ (or more generally position $\hat{X}$) of the central particle becomes linearly coupled to the position coordinates $\hat{q}_i$ of the surrounding oscillators. We weight each of these couplings with a constant c_i and thereby obtain an interaction Hamiltonian of the form

$$\hat{H}_{\text{int}} = \hat{\sigma}_z \otimes \sum_i c_i \hat{q}_i \equiv \hat{\sigma}_z \otimes \hat{E} \tag{4.4.3}$$

The assumption here of bilinear coupling (by which we mean linear coupling in both $\hat{\sigma}_z$ and $\hat{q}_i$) is important in determining the dynamics of our model. As such we refer to this explicitly as a "linear Spin-Boson model". All our subsequent work will be based on this assumption, since this is the most commonly studied model.

As we remarked earlier, when we first introduced decoherence, the form of the interaction determines the selected basis for decoherence and it is clear here that the interaction Hamiltonian causes environmental "monitoring" of the spin-basis of our system. As such, before any further calculations we may reasonably postulate that the interaction will cause decoherence in the spin-basis (or more generally in the position-basis of the untruncated system). This is not to say that this will be the sole effect of the interaction, we may expect to see dissipation and possibly even decoherence in other bases, although we anticipate that this would happen on a significantly larger timescale.

We begin by calculating the environment self-correlation functions which we note will hold for all harmonic-oscillator environments since they are independent of the central system. Since $\hat{H}_{\text{int}}$ is limited to only a single term, the only function we need compute is

$$C(\tau) = \langle \hat{E}(\tau)\hat{E} \rangle_{\hat{\varrho}_\varepsilon(0)} \tag{4.4.4}$$

Note here that in this chapter we will use the convention that all operators other than the density operator with explicit time arguments, are to be understood as interaction-picture operators. We may now insert equation (4.4.3) into this as well as writing $\hat{\varrho}_\varepsilon(0)$ as $\hat{\varrho}_\varepsilon$ to yield

$$C(\tau) = \sum_{i,j} c_i c_j \langle \hat{q}_i(\tau)\hat{q}_j \rangle_{\hat{\varrho}_\varepsilon} = \sum_i c_i^2 \langle \hat{q}_i(\tau)\hat{q}_i \rangle_{\hat{\varrho}_\varepsilon} \tag{4.4.5}$$

where the second equality here follows from the independence of oscillators under the general evolution generated by $\hat{H}$ as well as the fact that $\langle \hat{q}_i(\tau) \rangle = 0$. As earlier we have omitted the symbol $\otimes$ representing the tensor product between operators which pertain to separate fragments of the environment, and we will continue to do this throughout the chapter. Given this, an evaluation of $C(\tau)$ reduces simply to computing the averages $\langle \hat{q}_i(\tau)\hat{q}_i \rangle_{\hat{\varrho}_\varepsilon}$.

In order to facilitate this we switch our representation of $\hat{q}_i$ to that of the bosonic creation and annihilation operators $\hat{a}_i^\dagger$ and $\hat{a}_i$ respectively which are defined as

$$\hat{a}_i = \frac{1}{\sqrt{2m_i\omega_i}} \left(\hat{P}_i + im_i\omega_i\hat{q}_i \right)$$
$$\hat{a}_i^\dagger = \frac{1}{\sqrt{2m_i\omega_i}} \left(-\hat{P}_i + im_i\omega_i\hat{q}_i \right) \tag{4.4.6}$$

which give us the relations

$$\left[\hat{a}_i, \hat{a}_i^\dagger \right] = 1 \qquad\qquad \left[\hat{a}_i, \hat{a}_j^\dagger \right] = 0 \text{ for } i \neq j$$
$$\hat{H}_i = \frac{\omega_i}{2} \hat{a}_i^\dagger \hat{a}_i \tag{4.4.7}$$

readers who may be unfamiliar with these operators may wish to briefly consult a textbook, where any introductory textbook is likely to contain these operators. However along with spin and superpositions these are fairly standard content for a first course in quantum mechanics and as such I won't discuss them in detail. Using these operators we may clearly write

$$\hat{q}_i = \sqrt{\frac{1}{2m_i\omega_i}} \left(\hat{a}_i + \hat{a}_i^\dagger \right) \tag{4.4.8}$$

we note that,

$$\frac{d\hat{a}_i^\dagger}{dt} = i\left[\hat{H}_0, \hat{a}_i^\dagger \right] = i\omega_i \left[\hat{a}_i^\dagger\hat{a}_i, \hat{a}_i^\dagger \right] = i\omega_i\hat{a}_i^\dagger \tag{4.4.9}$$

which along with an analogous expression for $\hat{a}_i$ allows us to write the time-evolved state $\hat{q}_i(\tau)$ as

$$\langle \hat{q}_i(\tau)\hat{q}_i \rangle = \frac{1}{2m_i\omega_i} \langle \hat{a}_i\hat{a}_i^\dagger e^{-i\omega_i\tau} + \hat{a}_i^\dagger\hat{a}_i e^{i\omega_i\tau} \rangle_{\hat{\varrho}_\varepsilon}$$
$$= \frac{1}{2m_i\omega_i} \left\{ \langle \hat{a}_i\hat{a}_i^\dagger \rangle_{\hat{\varrho}_\varepsilon} e^{-i\omega_i\tau} + \langle \hat{a}_i^\dagger\hat{a}_i \rangle_{\hat{\varrho}_\varepsilon} e^{i\omega_i\tau} \right\} \tag{4.4.10}$$

From here we merely realize that $N_i = \langle \hat{a}_i^\dagger\hat{a}_i \rangle_{\hat{\varrho}_\varepsilon}$ is simply the mean occupation number of the ith oscillator in the environment. Given the assumption that the environment is in thermal equilibrium we obtain

$$N_i \equiv N_i(T) = \left(e^{\frac{\omega_i}{k_B T}} - 1 \right)^{-1} \tag{4.4.11}$$

Since we have followed much of the literature and set $\hbar = 1$ which allowed us to write the commutation relation $\left[\hat{a}_i, \hat{a}_i^\dagger \right]$ in equation (4.4.7), we express equation (4.4.10) as

$$\langle \hat{q}_i(\tau)\hat{q}_i \rangle_{\hat{\varrho}_\varepsilon} = \frac{1}{2m_i\omega_i} \left\{ [1 + N_i(T)] e^{-i\omega_i\tau} + N_i(T)e^{i\omega_i\tau} \right\}$$
$$= \frac{1}{2m_i\omega_i} \left\{ [1 + 2N_i(T)] \cos(\omega_i\tau) - i\sin(\omega_i\tau) \right\}$$
$$= \frac{1}{2m_i\omega_i} \left\{ \coth\left(\frac{\omega_i}{2k_B T} \right) \cos(\omega_i\tau) - i\sin(\omega_i\tau) \right\} \tag{4.4.12}$$

where this final equality comes from rewriting $1 + 2N_i(T)$ as

$$1 + 2\left(e^{\frac{\omega_i}{k_B T}} - 1 \right)^{-1} = \frac{e^{\frac{\omega_i}{k_B T}} + 1}{e^{\frac{\omega_i}{k_B T}} - 1} = \coth\left(\frac{\omega_i}{2k_B T} \right) \tag{4.4.13}$$

Therefore, we have expressed the environment self-correlation function as

$$C(\tau) = \sum_i \frac{c_i^2}{2m_i\omega_i} \left\{ \coth\left(\frac{\omega_i}{2k_BT}\right)\cos(\omega_i\tau) - i\sin(\omega_i\tau) \right\}$$
$$= \upsilon(\tau) - i\eta(\tau) \tag{4.4.14}$$

where we have the functions $\upsilon(\tau)$ and $\eta(\tau)$ defined as

$$\upsilon(\tau) = \frac{1}{2}\sum_i c_i^2 \langle \{\hat{q}_i(\tau), \hat{q}_i\}\rangle_{\hat{\varrho}_\varepsilon}$$
$$= \sum_i \frac{c_i^2}{2m_i\omega_i}\coth\left(\frac{\omega_i}{2k_BT}\right)\cos(\omega_i\tau)$$
$$= \int_0^\infty J(\omega)\coth\left(\frac{\omega_i}{2k_BT}\right)\cos(\omega_i\tau)d\omega \tag{4.4.15}$$

and

$$\eta(\tau) = \frac{i}{2}\sum_i c_i^2 \langle [\hat{q}_i(\tau), \hat{q}_i]\rangle_{\hat{\varrho}_\varepsilon}$$
$$= \sum_i c_i^2 \frac{1}{2m_i\omega_i}\sin(\omega_i\tau)$$
$$= \int_0^\infty J(\omega)\sin(\omega_i\tau)d\omega \tag{4.4.16}$$

where we have introduced the function $J(\omega)$ which is called the spectral density function. Before saying more about this function, we note that these functions are very important (in the next chapter they arise again entirely independently of this work when we solve the spin-boson model exactly) and are called the noise kernel and dissipation kernel respectively. Note that in equation (4.4.15) the curly brackets represent the anticommutator such that $\{A, B\} = AB + BA$. Returning to the spectral density function defined as

$$J(\omega) = \sum_i \frac{c_i^2}{2m_i\omega_i}\delta(\omega - \omega_i) \tag{4.4.17}$$

It is clear that the form of this function encapsulates the physical properties of the environment. We shall as a matter of course go to the continuum limit of the environment wherein we replace the discrete description in terms of individual oscillator frequencies (ω_i) and masses (m_i), by a continuous spectral density function which corresponds to a continuous spectrum of frequencies being present in the environment. However we shall temporarily stick to the representation of equation (4.4.17) for $J(\omega)$, which therefore, currently, merely allows a more compact expression for both $\upsilon(\tau)$ and $\eta(\tau)$.

We have thus determined the environment self-correlation function $C(\tau)$ thereby completing the hardest part of finding the Born-Markov master-equation for any harmonic oscillator-environment model with linear coupling. We may now express our operators B_α and C_α from equation (4.2.30) as

$$\hat{B}_\alpha = \int_0^\infty d\tau \sum_\beta C_{\alpha\beta}(\tau)\hat{S}_\beta^{(I)}(-\tau) = \int_0^\infty d\tau C(\tau)\hat{\sigma}_z(-\tau) \tag{4.4.18}$$

$$\hat{C}_\alpha = \int_0^\infty d\tau \sum_\beta C_{\alpha\beta}(-\tau)\hat{S}_\beta^{(I)}(-\tau) = \int_0^\infty d\tau C(-\tau)\hat{\sigma}_z(-\tau) \tag{4.4.19}$$

where,

$$\hat{\sigma}_z(\tau) = e^{i\hat{H}_s\tau}\hat{\sigma}_z e^{-i\hat{H}_s\tau} \tag{4.4.20}$$

is the spin-operator, representing position of the system in the right or left well, in the interaction picture. Combining all these terms we find the general expression for the Born-Markov master-equation as

$$\frac{d}{dt}\hat{\varrho}_s(t) = -i\left[\hat{H}_s, \hat{\varrho}_s(t)\right] - \int_0^\infty d\tau \left\{ \upsilon(\tau)\left[\hat{\sigma}_z, \hat{\sigma}_z(-\tau)\hat{\varrho}_s(t)\right] + C(-\tau)\left[\hat{\varrho}_s(t)\hat{\sigma}_z(-\tau), \hat{\sigma}_z\right] \right\} \tag{4.4.21}$$

Which, when we insert the decomposition $C(\tau) = \upsilon(\tau) - i\eta(\tau)$ and note $\upsilon(-\tau) = \upsilon(\tau)$ and $\eta(-\tau) = -\eta(\tau)$ we rearrange into the final form for our Born-Markov master equation,

$$\frac{d}{dt}\hat{\varrho}_s(t) = -i\left[\hat{H}_s, \hat{\varrho}_s(t)\right] - \int_0^\infty d\tau \left\{ \upsilon(\tau)\left[\hat{\sigma}_z, \left[\hat{\sigma}_z(-\tau), \hat{\varrho}_s(t)\right]\right] - i\eta(\tau)\left[\hat{\sigma}_z, \{\hat{\sigma}_z(-\tau), \hat{\varrho}_s(t)\}\right] \right\} \tag{4.4.22}$$

As a result of this we finally remark that decoherence (and dissipation) is entirely described by integrals over the noise and dissipation kernels as defined in (4.4.15) and (4.4.16), multiplied by varying products of spin-operators of the system (in both the Schrödinger and interaction-picture).

We now turn to a more careful analysis of equation (4.4.22). Once we introduce the self-Hamiltonian we have a complete Hamiltonian of the form

$$\hat{H} = \frac{1}{2}\varepsilon\hat{\sigma}_z - \frac{1}{2}\Delta_0\hat{\sigma}_x + \sum_i \left(\frac{1}{2m_i}\hat{P}_i^2 + \frac{1}{2}m_i\omega_i^2\hat{q}_i^2 \right) + \hat{\sigma}_z \otimes \sum_i c_i\hat{q}_i \tag{4.4.23}$$

where Δ_0 is the bare-tunneling amplitude and ε is the "asymmetry energy" (as shown in Fig.6). In the next chapter we provide a reasonably lengthy motivation for each term in this Hamiltonian and Leggett et al. [3] justified it rigorously purely from physical considerations. However, here we simply assume that such a Hamiltonian is applicable and further we set the "asymmetry energy" ε equal to zero, so that we are considering the unbiased case.

We may solve the time-dependence of the operator $\hat{\sigma}_z$ in the interaction picture by solving the Heisenberg equations of motion with respect to $\hat{H}_s$. the result of such a calculation is

$$\frac{d}{d\tau}\hat{\sigma}_z(\tau) = i\left[\hat{H}, \hat{\sigma}_z\right] = -\frac{1}{2}\Delta_0\hat{\sigma}_y$$
$$\frac{d^2}{d\tau^2}\hat{\sigma}_z(\tau) = i\left[\hat{H}, i\left[\hat{H}, \hat{\sigma}_z\right]\right] = -\left(\frac{\Delta_0}{2}\right)^2\hat{\sigma}_z \tag{4.4.24}$$

which allows us to solve as

$$\hat{\sigma}_z(\tau) = \hat{\sigma}_z \cos\left(\frac{\Delta_0}{2}\tau\right) - \hat{\sigma}_y \sin\left(\frac{\Delta_0}{2}\tau\right) \tag{4.4.25}$$

We continue by substituting this equation into the right-hand side of our master-equation (4.4.22) to obtain

$$-i\left[\hat{H}_s, \hat{\varrho}_s(t)\right] - \int_0^\infty d\tau \ \upsilon(\tau)\cos\left(\frac{\Delta_0\tau}{2}\right)[\hat{\sigma}_z, [\sigma_z, \hat{\varrho}_s(t)]] + \upsilon(\tau)\sin\left(\frac{\Delta_0\tau}{2}\right)[\hat{\sigma}_z, [\hat{\sigma}_y, \hat{\varrho}_s(t)]]$$
$$- i\eta(\tau)\cos\left(\frac{\Delta_0\tau}{2}\right)[\hat{\sigma}_z, \{\hat{\sigma}_z, \hat{\varrho}_s(t)\}] + i\eta(\tau)\sin\left(\frac{\Delta_0\tau}{2}\right)[\hat{\sigma}_z, \{\hat{\sigma}_y, \hat{\varrho}_s(t)\}] \tag{4.4.26}$$

where we can now clearly set the term $[\hat{\sigma}_z, \{\hat{\sigma}, \hat{\varrho}_s(t)\}]$ equal to zero. We assign symbol for the functions

$$\tilde{D} \equiv \int_0^\infty d\tau\upsilon(\tau)\cos\left(\frac{\Delta_0\tau}{2}\right) \tag{4.4.27}$$

$$\tilde{f} \equiv \int_0^\infty d\tau\upsilon(\tau)\sin\left(\frac{\Delta_0\tau}{2}\right) \tag{4.4.28}$$

$$\tilde{\gamma} \equiv \int_0^\infty d\tau\eta(\tau)\sin\left(\frac{\Delta_0\tau}{2}\right) \tag{4.4.29}$$

and through more trivial rearrangement we ultimately express our master-equation as

$$\frac{d}{dt}\hat{\varrho}_s(t) = -i\left(\hat{H}_s'\hat{\varrho}_s(t) - \hat{\varrho}_s(t)\hat{H}_s'^\dagger\right) - \hat{D}\left[\hat{\sigma}_z\left[\hat{\sigma}_z, \hat{\varrho}_s(t)\right]\right] + \zeta\hat{\sigma}_z\hat{\varrho}_s(t)\hat{\sigma}_y + \zeta^*\hat{\sigma}_y\hat{\varrho}_s(t)\hat{\sigma}_z \tag{4.4.30}$$

as given in Ch.5 of [26], where we have here defined the perturbed (possibly non-Hermitian) Hamiltonian $\hat{H}_s'$ as,

$$\hat{H}_s' = \left(-\frac{1}{2}\Delta_0 - \zeta^*\right)\hat{\sigma}_x \tag{4.4.31}$$

which corresponds to a renormalization of energy levels (Lamb-shift) by an amount

$$\zeta^* = \tilde{f} - i\tilde{\gamma} \tag{4.4.32}$$

the coefficients $\tilde{D}$, $\tilde{f}$ and $\tilde{\gamma}$ are called respectively the normal-diffusion coefficient, the anomalous diffusion coefficient and the damping coefficient. We concentrate on the term

$$\tilde{D}\left[\hat{\sigma}_z, [\hat{\sigma}_z, \hat{\varrho}_s(t)]\right] \tag{4.4.33}$$

which while begin of the standard Lindblad double-commutator form is the term which represents direct monitoring of the observable $\hat{\sigma}_z$ by the environment. As such it describes decoherence into the $\{|0\rangle, |1\rangle\}$-basis at a rate dictated by $\tilde{D}$.

To see this more clearly we express the term as a matrix in the basis $\{|0\rangle, |1\rangle\}$, by denoting the matrix elements $\langle i|\hat{\varrho}_s(t)|j\rangle$ as $\hat{\varrho}_s^{(ij)}(t)$ we get,

$$\tilde{D}\left[\hat{\sigma}_z, [\hat{\sigma}_z, \hat{\varrho}_s(t)]\right] = \tilde{D}\begin{pmatrix} 0 & \varrho_s^{(01)}(t) \\ \varrho_s^{(10)}(t) & 0 \end{pmatrix} \tag{4.4.34}$$

which is easily derived from the Pauli spin-$\frac{1}{2}$ matrices. As such the evolution of the off-diagonal elements within our reduced density matrix due to the $\tilde{D}$ term alone is

$$\frac{d}{dt}\varrho_s^{(01)}(t) = -\tilde{D}\varrho_s^{(01)}(t)$$
$$\frac{d}{dt}\varrho_s^{(10)}(t) = -\tilde{D}\varrho_s^{(10)}(t) \tag{4.4.35}$$

This indicates that the off-diagonal elements decay due to the term $\tilde{D}$ at a rate exponentially proportional to $\tilde{D}$, whereas the diagonal elements remain unaffected, which indicates a pure decoherence process without damping. Since our focus here is on decoherence we shall not examine the role of the other coefficients and instead continue to solve the spin-boson model exactly and thus examine dissipation, damping and other processes that way. The main weakness of our above work is the assumption that the environment behaves in a Markovian fashion. In the next chapter we do not make such an assumption and the result is much richer dynamics.

4.5 Summary

- We first discussed a very general form for the master-equation decomposed into a unitary part with reference to $\hat{H}_S^{'}$ and a non-unitary part $\hat{D}$ as,
$$\frac{d}{dt}\hat{\varrho}_s(t) = -i\left[\hat{H}_S^{'}, \hat{\varrho}_s(t)\right] + \hat{D}\left[\hat{\varrho}_s(t)\right] \tag{4.5.1}$$

- We decomposed the Hamiltonian into the self and interaction parts and then switched to the interaction picture and solved exactly to the point
$$\frac{d}{dt}\hat{\varrho}_s^{(I)}(t) = -\int_0^t dt^{'}\,\mathrm{Tr}_\varepsilon\left[\hat{H}_{\mathrm{int}}(t), \left[\hat{H}_{\mathrm{int}}(t^{'}), \hat{\varrho}^{(I)}(t^{'})\right]\right] \tag{4.5.2}$$

- We make two requirements of our master-equation: that it is local in time and depends only on $\hat{\varrho}_s(t)$ and $\hat{\varrho}_\varepsilon(0)$ and other known quantities.

- To these ends we impose the Born Approximation motivated by weak interaction between system and environment alongside the environment being large compared to the system. We then introduce the approximation as
$$\hat{\varrho}(t) \approx \hat{\varrho}_s(t) \otimes \hat{\varrho}_\varepsilon(0) \tag{4.5.3}$$

- The second approximation is the Markov Approximation which is motivated by sufficiently weak connection between the system and environment and the environment being of a sufficiently high temperature that it's evolution is sufficiently quick. As such, this assumption is much more limiting than that of the Born approximation which we expect to hold whenever the envionment is macroscopic. The Markov Assumption allows us to set our self-correlation functions to be time local since they decay very rapidly.

- This all allows us to write our Born-Markov master-equation in the form

$$\frac{d}{dt}\hat{\varrho}_s(t) = -i\left[\hat{H}_s, \hat{\varrho}_s(t)\right] - \int_0^\infty d\tau \left\{C_{\alpha\beta}(\tau)\left[\hat{S}_\alpha, \hat{S}_\beta(-\tau)\hat{\varrho}_s(t)\right] + C_{\beta\alpha}(-\tau)\left[\hat{\varrho}_s(t)\hat{S}_\beta(-\tau), \hat{S}_\alpha\right]\right\} \tag{4.5.4}$$

- We next introduced the idea of Canonical Models and discussed 'mappings' in the case of continuous and discrete variables.

- We discussed the possible relevant scenarios for spin-particles and oscillators to represent either the system or environment and specifically mentioned that for 'sufficiently weak' interaction the environment can always be modelled as a collection of Harmonic Oscillators.

- We continued by deriving the Born-Markov master-equation for the Linear Spin-Boson Model.

- We did this by expressing the environment self correlation functions $C(\tau)$ in terms of $\nu(\tau)$ and $\eta(\tau)$ the noise and dissipation kernels respectively which themselves are functions of the spectral density function $J(\omega)$.

- We wrote out our master-equation and briefly analyzed each of the terms found on the right-hand side and the role each one plays in terms of decoherence, dissipation and other processes.

5 Exact Expressions for the System Dynamics and the Non-Interacting Blip Approximation

As discussed last chapter, the implementation of the Markov Approximation is currently the most limiting factor in our model. We expect this approximation to hold in 'everyday settings', however it is not these settings where most of our cases of interest arises. Indeed we remarked in the first section on Canonical Models, that a central system being modelled as a spin-$\frac{1}{2}$ particle often arises as a result of low temperatures. In quantum computing, in order that we may minimize the destructive influence of decoherence on our states, experimenters 'freeze' out the thermal environment, all of which means that in such cases of interest the Markov Approximation is not a priori justified.

However it is a miraculous result that the Spin-Boson model can be solved precisely in certain regimes and that is the task we now undertake. We hope that from this we can obtain a full expression for the dynamics of the Spin-Boson model which is more widely applicable than the Born-Markov master-equation and from this we could obtain values such as decoherence timescales and dissipation timescales. Ultimately however we will be most concerned with those regions for which the Markov approxiamtion is least applicable and therefore possibly give qualitatively different results from those of our master-equation. We will discuss the dynamics for the less stringent Markov condition called the Non-Interacting Blip Approximation, however due to restrictions in space and time a similar analyis of the dynamics in the case of the Born-Markov master-equation derived last chapter will be left to the reader. Suffice to say that the model derived in the next two chapters is more precise, more rigorously justified and much more applicable in the regimes of dissipation and temperature for which our earlier results fall away. A good place to start for an analysis of the Born Markov master-equation for the Spin-Boson model would be Ch.5 of [26]. Bearing this in mind we begin to address the model, starting with a justification for the Hamiltonian we are using.

5.1 Formulation of the Problem

Leggett et al. [3] derived the Hamiltonian for the Spin-Boson model from entirely physical considerations, however we will restrict ourselves to a general motivation for the form of the Hamiltonian. We decompose the Hamiltonian into three constituent parts, the self-Hamiltonians for the system and the environment as well as a Hamiltonian representing the interaction between the two. The system's Hamiltonian is comprised of two parts, firstly a tunneling term and secondly a term coming from ε, the so-called "detuning parameter", which as can be seen from Fig.6 is the bias between the ground-state energies. Therefore

$$\hat{H}_S = -\frac{1}{2}\Delta\hat{\sigma}_x + \frac{\varepsilon}{2\hbar}\hat{\sigma}_z \tag{5.1.1}$$

where $\hat{\sigma}_x$ and $\hat{\sigma}_z$ are the Pauli-spin matrices and Δ is the "bare" tunneling matrix element. We assume that the correlations which are established between the oscillators which constitute the environment are negligible, i.e. that the oscillators evolve independently. This leaves the environment self-Hamiltonian as simply the sum of the self-Hamiltonians of the constituent oscillators

$$\hat{H}_\varepsilon = \frac{1}{\hbar}\sum_\alpha\left(\frac{1}{2}m_\alpha\omega_\alpha^2\hat{\chi}_\alpha^2 + \frac{\hat{P}_\alpha^2}{2m_\alpha}\right) \tag{5.1.2}$$

where $\hat{\chi}_\alpha$, m_α, $\hat{P}_\alpha$ and ω_α are the position co-ordinate, mass, momentum co-ordinate and frequency of the αth oscillator respectively. This leaves us to consider the interaction Hamiltonian, we expect coupling to occur between the position co-coordiantes of both system and oscillators with coupling coefficients C_α. As can be seen from Fig.6 the position of the system is given as $\frac{1}{2}q_0\hat{\sigma}_z$. Therefore we express the interaction Hamiltonian in the form

$$\hat{H}_{\text{int}} = \frac{q_0}{2\hbar}\hat{\sigma}_z \otimes \sum_\alpha C_\alpha\hat{\chi}_\alpha \tag{5.1.3}$$

where we subsequently omit the tensor product symbol $\otimes$. Putting these Hamiltonians together, we obtain

$$\hbar\hat{H} = -\frac{1}{2}\hbar\Delta\hat{\sigma}_x + \frac{1}{2}\varepsilon\hat{\sigma}_z + \sum_\alpha\left(\frac{1}{2}m_\alpha\omega_\alpha^2\hat{x}_\alpha^2 + \frac{\hat{p}_\alpha^2}{2m_\alpha}\right) + \frac{1}{2}q_0\hat{\sigma}_z\sum_\alpha C_\alpha\hat{x}_\alpha \tag{5.1.4}$$

In truncating the double-well potential certain limits were imposed by Leggett et al. [3] and to be consistent we must observe these in our subsequent work. These limits are $\frac{\Delta}{\omega_c}$, $\frac{kT}{\hbar\omega_c}$ and $\frac{\varepsilon}{\hbar\omega_c} \ll 1$ where ω_c is an arbitrarily chosen high-frequency cutoff for the frequencies of the oscillators. From this point on we accept that these limits are sufficient to allow us to use the Hamiltonian

We start by defining

$$J(\omega) = \frac{\pi}{2}\sum_\alpha\frac{C_\alpha^2}{m_\alpha\omega_\alpha}\delta(\omega - \omega_\alpha) \tag{5.1.5}$$

This $J(\omega)$ is called the spectral density and as such has a high-frequency cut-off of order ω_c, such a high-frequency cutoff is to be expected since no environment has unbounded frequencies.Iin order to be consistent with the derivation of (5.1.4) we may assume ω_c is large compared to Δ. It is worth mentioning that the exact expressions here derived do not rely on

$\frac{\Delta}{\omega_c} \ll 1$, however the behaviours later described for the ohmic case are in general valid only to non-trivial order in $\frac{\Delta}{\omega_c}$, $\frac{kT}{\hbar\omega_c}$, and $\frac{\varepsilon}{\hbar\omega_c}$.

We shall from here on make the assumption that the spectral density can be considered a continuous and fairly smooth function. This implies that the spectrum of oscillator frequencies ω_α can be considered dense enough, i.e., that we have sufficiently large environment we may consider a continuous representation of all frequencies at least as high as ω_c, our high-frequency cut-off. We also require that the distribution of masses m_α and coupling constants C_α are not overly pathological in such a way as to break this assumption.

We shall restrict our attention to the situation where the spectral density function $J(\omega)$ of the original (untruncated) system has a power-law form for $\omega \lesssim \omega_c$:

$$J(\omega) = A\omega^s e^{-\frac{\omega}{\omega_c}} \tag{5.1.6}$$

with $A\epsilon\mathbb{R}$ being a constant. The special case we will later specialise in is known as 'ohmic dissipation' (so named for historical rather than illustrative reasons), which refers to the situation where in (5.1.6) $s = 1$, $A = \eta$. For this instance we define a dimensionless measure of the system-environment coupling,

$$\alpha \equiv \eta \frac{q_0^2}{2\pi\hbar} \tag{5.1.7}$$

which (importantly) is independent of the value of our chosen high-frequency cut-off ω_c. This is especially useful since it allows us to utilise α and $\frac{\Delta}{\omega_c}$ as two formally independent dimensionless parameters with which to describe our problem. This useful characteristic of our dimensionless system-environment coupling is unique to the ohmic case, since in the non-ohmic case (i.e. where $s \neq 1$) the definition of such a coupling requires reference to some frequency scale. For this and other reasons we will restrict our attention to the ohmic case and not the subohmic ($s < 1$) or superohmic ($s > 1$) cases.

Let us consider precisely which features of this model we would like to investigate since, for example, we have no interest in the environment for its own sake, we are merely interested in its effect on our system of interest. As such, we intend to impose some feasible and justifiable initial conditions on the system and environment, then investigate the expectation values of variables which can be measured on the system at some later time. However, we ideally do not want to have to refer to our environment at these times, since for any reasonably large environment with many degrees of freedom this information is unlikely to be practically accessible and so, as before, we will trace over the environmental states. We consider only the variable $\hat{\sigma}_z$, which you will recall from our last chapter refers to the position being either in the left-well at $-\frac{q_0}{2} \equiv -1$ or in the right-well $\frac{q_0}{2} \equiv +1$. This is reasonable since in the majority of cases of practical interest it is only this variable which is directly measured.

We now ask two questions, by which we hope to capture the dynamics of the evolution, of the dissipative two-state system:

1. For $t < 0$ we hold the system at (say) the position $q = \frac{1}{2}q_0$ (meaning $\hat{\sigma}_z = +1$), while assuming that thermal equilibrium has been reached between the system and environment. At time $t = 0$, the constraint is released, meaning that for $t > 0$ the dynamics are governed by our Hamiltonian (5.1.4). We now wish to know, under these conditions, what is the subsequent expectation value of $\hat{\sigma}_z$ as a function of time, t? We shall call this quantity $P(t)$, and from such a quantity we could deduce dissipation and decoherence timescales with which to compare to those predicted by the Born-Markov master equation.

2. What is the symmetrized equilibrium correlation function

$$C(t) = \frac{1}{2}\langle\{\hat{\sigma}_z(t), \hat{\sigma}_z(0)\}\rangle_\beta \equiv \frac{1}{2Z}Tr[e^{i\hat{H}t/\hbar}\hat{\sigma}_z e^{-i\hat{H}t/\hbar}\hat{\sigma}_z e^{-\beta\hbar} + (t \rightarrow -t)] \tag{5.1.8}$$

where $\hat{H}$ is the complete Hamiltonian (5.1.4) and $Z(\beta)$ the partition function $\text{Tr}(e^{-\beta\hat{H}})$. This measures the correlation between $\hat{\sigma}_z$ at time t and the initial value, and as such clearly depends on how we define our initial conditions. From this quantity we may deduce the timescale on which the initial data is lost in the evolution, this would be due to a combination of dissipation and decoherence along with possibly other processes.

There are certainly many other questions which could be asked as well as variants on the initial condition in question (1), however, it is clear why both of these are important questions to be asked.

We now derive explicit and exact formal expressions in the form of power series in Δ, for the quantity $P(t)$ and indicate an analogous method for $C(t)$. These solutions will be expressed, as expected, with respect to the spectral function $J(\omega)$ (5.1.5) and most importantly is valid independently of the form that we may later impose on $J(\omega)$. In particular, as mentioned earlier, the results here derived do not depend on our assumption $\Delta \ll \omega_c$. Having done this, we will consider an approximation, which for reasons that will become apparent, is called the Non-Interacting Blip approximation. Such an approximation is very useful, since as shall now be shown although we may obtain exact expressions, they are prohibitively complex.

5.2 Formal Expression for $P(t)$

We are considering a case where the environment consists entirely of harmonic oscillators, which we want to 'remove' from the problem, by which we mean remove them explicitly, while maintaining their influence. In this paper we use the "influence-functional" method as devised by Feynman and Vernon (1963) [23], using this we explicitly derive equations for a quantity

equivalent to $P(t)$. Our new formulation for $P(t)$ we will call $P'(t)$ imagines that at time $t = -\infty$ the system and environment are separately at thermal equilibrium. For some large negative time t_0 we "activate" the system-environment interaction, however with the constraint $\hat{\sigma}_z = +1$ maintained until $t = 0$ at which point we release this constraint. We now ask, in the limit $t_0 \to -\infty$, what is $< \hat{\sigma}_z >$ as a function of t for $t > 0$? Since an environment of N harmonic oscillators is not an ergodic environment it is non-trivial to show that these two prescriptions for $P(t)$ coincide for $t > 0$. However, Appendix B of [3] demonstrates that in our regime of interest $P(t) = P'(t) \forall t > 0$.

So, returning to the influence-functional method, we consider at an initial negative time $t_0 < 0$ a system with a time-dependent variable we call $x(\tau)$ starts with a value x_i and we postulate that the environment starts in a state of thermal equilibrium, that is with respect to its self-Hamiltonian. The work of Feynman and Vernon [23] then tells us that the probability, which we will denote $p(x_f; t)$ for the system to be present at x_f at time t, irrespective of environmental conditions at this time is given as

$$p(x_f; t) = \int Dx(\tau) \int Dy(\tau') A[x(\tau)] A^*[y(\tau')] F[x(\tau), y(\tau')] \tag{5.2.1}$$

where $D(x(\tau))$ denotes a double-path integral running over all possible paths denoted $x(\tau)$, $y(\tau')$ under the constraints $x(t_0) = y(t_0) = x_i$ and $x(t) = y(t) = x_f$. $A[x(\tau)]$ is the path-integral amplitude associated to each path $x(\tau)$, and the expression $F[x(\tau), y(\tau')]$ is the so-called influence-functional. In our case we can strengthen our constraint on paths, since we know that $x(\tau) = y(\tau) = x_i$ for all $t \leq 0$. It is worth mentioning straight away that these strengthened constraints do not lead simply to a truncated problem where we can limit ourselves to considering only $t > 0$. We cannot neglect the negative-time parts of the path, since their contribution to (5.2.1) continues in the form of their effects on the positive-time behaviour, as we shall later see.

It is an invaluable result to us that when an environment consists of harmonic oscillators, we are able to calculate the influence-functional exactly (see Feynman and Vernon 1963 [23]). We give it in the form

$$F[x(\tau), y(\tau')] = exp\left\{-\frac{1}{\hbar} \int_{t_0}^{t} d\tau \int_{t_0}^{\tau} ds [x(\tau) - y(\tau)][\gamma(\tau - s)x(s) - \gamma^*(\tau - s)y(s)]\right\} \tag{5.2.2}$$

where $\gamma(\tau - s)$ is defined as,

$$\gamma(\tau - s) \equiv \sum_{\alpha} \frac{C_\alpha^2}{2m_\alpha \omega_\alpha}\left[exp\left\{-\omega_\alpha(\tau - s)\right\} + \frac{2\cos(\omega_\alpha(\tau - s))}{exp\left\{\beta\hbar\omega_\alpha\right\} - 1}\right] \tag{5.2.3}$$

Recalling our definition (5.1.5) for $J(\omega)$ and taking the limit of integration, we find

$$\gamma(\tau - s) = \frac{1}{\pi} \int_0^\infty d\omega J(\omega)\left[e^{-i\omega(\tau - s)} + \frac{2\cos(\omega_\alpha(\tau - s))}{exp\left\{\beta\hbar\omega_\alpha\right\} - 1}\right] \tag{5.2.4}$$

we now proceed to simplify this equation, by rewriting the term inside the brackets,

$$e^{-i\omega(\tau - s)} + \frac{2\cos(\omega_\alpha(\tau - s))}{exp\left\{\beta\hbar\omega\right\} - 1} = -i\sin(\omega(\tau - s)) + \cos(\omega(\tau - s))\left(1 + \frac{2}{exp\left\{\beta\hbar\omega\right\} - 1}\right)$$

$$= -i\sin(\omega(\tau - s)) + \cos(\omega(\tau - s))\left(\frac{exp\left\{\beta\hbar\omega\right\} + 1}{exp\left\{\beta\hbar\omega\right\} - 1}\right)$$

$$= -i\sin(\omega(\tau - s)) + \cos(\omega(\tau - s))\coth\left(\frac{\beta\hbar\omega}{2}\right) \tag{5.2.5}$$

This motivates our next two definitions, namely:

$$L_1(\tau - s) = \int_0^\infty d\omega J(\omega)\sin(\omega(\tau - s)) \tag{5.2.6}$$

$$L_2(\tau - s) = \int_0^\infty d\omega J(\omega)\cos(\omega(\tau - s))\coth\left(\frac{\beta\hbar\omega}{2}\right) \tag{5.2.7}$$

which allows us in turn to write $\gamma(\tau - s)$ in terms of these functions as

$$\pi\gamma(\tau - s) = -iL_1(\tau - s) + L_2(\tau - s) \tag{5.2.8}$$

and using these results we rewrite our influence-functional in terms of $L_1(\tau - s)$ and $L_2(\tau - s)$. A simple reordering of terms yields the result:

$$F[x(\tau) - y(\tau)] = exp\left\{\frac{1}{\pi\hbar} \int_{t_o}^{t} d\tau \int_{t_0}^{\tau} ds \left(-iL_1(\tau - s)[x(\tau) - y(\tau)] \cdot [x(s) + y(s)] + L_2(\tau - s)[x(\tau) - y(\tau)] \cdot [x(s) - y(s)]]\right)\right\} \tag{5.2.9}$$

We now return our attention to the paths $x(\tau)$ and $y(\tau')$ in the two-state problem and recall that $x(\tau)$ and $y(\tau')$ are limited to two discrete values $\pm\frac{1}{2}q_0$. As such (5.2.1) can be considered as describing an integral over all possible pairs of

46

paths, where both paths oscillate between the two states, which is equivalent to considering a single path which travels between 4-states. Since in the path integral τ, τ', x and y are dummy indices we can entirely characterize the pair of paths if we specify at each time τ the pair $\{x(\tau), y(\tau)\}$. We denote the respective states as $\{+,+\} = A$, $\{+,-\} = B$, $\{-,+\} = C$, $\{-,-\} = D$, (where $+ \equiv \frac{1}{2}q_0$, etc.)

We now define two functions as:

$$\xi(\tau) \equiv q_0^{-1}[x(\tau) - y(\tau)]$$
$$\chi(\tau) \equiv q_0^{-1}[x(\tau) + y(\tau)] \tag{5.2.10}$$

where it is clear $\xi(\tau) = 0$ for states A and D, $\xi(\tau) = +1$ for state B and $\xi(\tau) = -1$ for state C, whereas $\chi(\tau) = 0$ for states B and C, $\chi(\tau) = +1$ for state A and finally $\chi(\tau) = -1$ for state D. Using these new functions we rewrite (5.2.9) as,

$$F[x(\tau) - y(\tau)] = exp\left\{-\frac{q_0^2}{\pi\hbar}\int_{t_0}^{t}d\tau\int_{t_0}^{\tau}ds[-iL_1(\tau-s)\xi(\tau)\chi(s) + L_2(\tau-s)\xi(\tau)\xi(s)]\right\} \tag{5.2.11}$$

Since it is evident from our definition of $\xi(\tau)$ that for all times $\tau < 0$, $\xi(\tau) = 0$, we take the lower limit of integration over τ to be zero. If we consider the states A and D, it is intuitively clear that they correspond to the diagonal elements of the reduced density matrix and B and C correspond to the off-diagonal terms.

Turning our attention to the $A[x(\tau)]$ term, we begin by assuming, for definiteness, that the state occupied for $t < 0$ was $+\frac{1}{2}q_0$ (i.e. the four-state path was in A). We also choose the zero of energy such that this state has energy $\frac{\varepsilon}{2}$ (where the sign of ε is as yet undetermined). If we break the total bare amplitude into pieces of length dt, then we can show the amplitude to stay in $+\frac{1}{2}q_0$ $(-\frac{1}{2}q_0)$ during this time interval dt is $= e^{[-i\left(\frac{\varepsilon}{2\hbar}\right)dt]}$ $(e^{[i\left(\frac{\varepsilon}{2\hbar}\right)dt]})$. Similarly, the amplitude for a switch in states is given by $i\left(\frac{\Delta}{2}\right)dt$, and this is valid in either direction. If we directly substitute these formulations into our four-state path and initially limit our consideration to paths with only a single flip (i.e. ignore those which follow a path of the form $1 \to 2 \to 1$ or similar), then we obtain simple amplitudes. The amplitude for remaining in the same four-state is $exp[-i\,\varepsilon\,\xi(t)dt]$, or for switching between states is $i\lambda\left(\frac{\Delta}{2}\right)dt$, where λ is defined as,

$$\lambda = \begin{cases} = 0 & A \rightleftharpoons D, B \rightleftharpoons C \\ = -1 & A \rightleftharpoons B, C \rightleftharpoons D \\ = +1 & A \rightleftharpoons C, B \rightleftharpoons D \end{cases} \tag{5.2.12}$$

which accounts for the inability to switch simultaneously both states e.g. $\{+,+\} \rightleftharpoons \{-,-\}$ without passing through B or C. Equally, since our equation has the terms $A[x(\tau)]A^*[y(\tau')]$ if the $y(\tau)$ path changes we get a term $-i\left(\frac{\Delta}{2}\right)dt$ by the complex conjugation, this is now also dealt with by the λ. Therefore the role of λ can be shown diagrammatically by
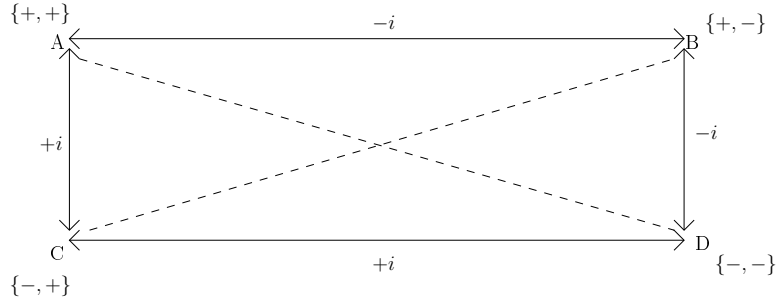

Figure 7: A diagrammatical representation of the role of the variable λ

If we consider a definite 4-state path that is initially in state A and also in A at time t, making $2n$-transitions (i.e. flips) during this time. Consider from Fig.7 above that any two jumps from $A \rightleftharpoons D$ results in a $+1$, and any two jumps which go from $A \to A$ or $D \to D$ result in a -1. We use these facts to claim that any path of 2n-jumps has a term of the form $(-1)^n \left(\frac{\Delta}{2}\right)^{2n}$. Firstly the second part of this equation, namely $\left(\frac{\Delta}{2}\right)^{2n}$ is obviously a result of 2n-transistions each one bringing a factor of the form $\frac{\Delta}{2}$. As such we now merely need to consider the $(-1)^n$ part, since we begin at and return to A, any pair of jumps from $A \to D$, must have another pair of jumps which we can complete the loop from $D \to A$. If we combine these into sets of 4-jumps, then it is clear that these contribute $+1$ since each 2-step path between these states contributes a $+1$ and in our equation this would give $(-1)^{\frac{1}{2}4} = 1$. This now leaves us with m transition-pairs from A to itself or from D to itself. Each of these contributes a factor of -1 and since any path can be constructed as the union of such transition-pairs with the previously mentioned loops the factor we have the resulting factor $(-1)^{\frac{1}{2}2m}$. This doesn't match our equation perfectly, but since $(-1)^{m+2a} \equiv (-1)^m$ for any integer a, then these formulae are equivalent. As such we have $2m + 4a$ jumps where the m-jumps are from $A \to A$ or $D \to D$ and the a jumps are loops from A to itself, which yields our result, proving our claim.

47

We next use the fact that each "odd-flip" (i.e. first , third etc.) takes us to state B or C and each "even-flip" leaves us in either state A or D, except of course for the $2n^{\text{th}}$ flip which necessarily leaves us back in state A. Bearing this in mind we define two new variables, if we consider a particular path where the mth transition occurs at a time denoted t_m, then we assign every interval of the form $t_{2j-1} < t < t_{2j}$ the variable ζ_j, which is +1 (-1) if the system resides in state B (state C) during this period. Similarly we define η_j in the interval $t_{2j} < t < t_{2j+1}$ as +1 (-1) if it's in state A (state D) and note that by construction we have $\eta_0 \equiv \eta_n \equiv +1$. These prescriptions allow us to evaluate our influence functional (5.2.11) for any paths as a function which we will denote $\tilde{F}_n$ of the quantities $\{t_m\}$, $\{\zeta_i\}$ and $\{\eta_i\}$. We also choose for convenience to incorporate the asymmetry factor $\exp[-i\varepsilon \int_0^t \xi(t)dt]$. The probability $p(t)$ which we have been aiming for is therefore expressed as a series in Δ^2,

$$p(t) = 1 + \frac{1}{2}\sum_{n=1}^{\infty}(-1)^n \Delta^{2n} K_n(t) \tag{5.2.13}$$

$$K_n(t) = 2^{-(2n-1)} \sum_{\{\zeta_j, \eta_j\}} \int_0^t dt_{2n} \int_0^{t_{2n}} dt_{2n-1}... \int_0^{t_2} dt_1 \tilde{F}_n(t_1, t_2, ...t_{2n-1}, \zeta_1, ..., \zeta_n, \eta_1, ...\eta_{n-1}) \tag{5.2.14}$$

where we have yet to find an expression for $\tilde{F}_n$. Note we have done several small changes in writing these last two equations, which while simple, they may be cumulatively be misleading and so we will identify changes with several remarks. The '1' in (5.2.13) represents the zero-transition case. The $\frac{1}{2}$ before our sum in this equation joins with the $2^{-(2n-1)}$ from (5.2.14) to give us the 2^{-n} from before, we have chosen this form as it is conducive to our next step. The sum over $\{\zeta_j\}$ and $\{\eta_j\}$ in (5.2.14) ensures that every path is considered, since these variables now dictate which state the system is in. Finally note that the form of our time integrals vary over all possible times for our transitions, while still ensuring $t_1 < t_2 < t_3...$, i.e. we have $2n$ mutually exclusive integrals.

If we now use this expression for $p(t)$ to obtain an expression for $\langle\hat{\sigma}_z(t)\rangle$ we have $P(t) = \langle\hat{\sigma}_z(t)\rangle = (p(t) \cdot (1) + ((1-p(t)) \cdot (-1)) = 2p(t) - 1$ giving,

$$P(t) = \sum_0^{\infty}(-1)^n \Delta^{2n} K_n(t) \tag{5.2.15}$$

where $K_0(t)$ is by definition equal to one. Let us briefly consider a pictorial representation of our two paths in order that we may highlight some pertinent variables that we will continually make reference to.
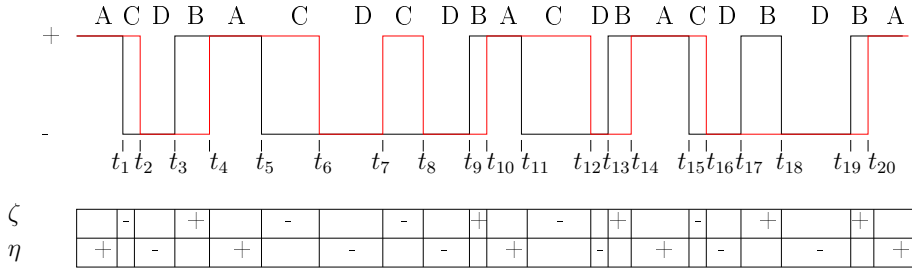

Figure 8: A Diagram representing an example of a four-state path with some of the pertinent values and variables shown. (Note that later we will use a similar form of representation that is importantly distinct and that elsewhere in the literature such diagrams are usually those the reader is likely to encounter).

So, now we consider finding an expression for our functions $\tilde{F}_n$. To this end we define our functions, using the heavyside step function $\theta(t)$, as

$$\chi(\tau) = \sum_{j=o}^{n} \eta_j[\theta(\tau - t_{2j}) - \theta(\tau - t_{2j+1})] \tag{5.2.16}$$

$$\xi(\tau) = \sum_{j=1}^{n} \zeta_j[\theta(\tau - t_{2j-1}) - \theta(\tau - t_{2j})] \tag{5.2.17}$$

The role of (5.2.16) is that if $\tau \in [t_{2j}, t_{2j+1}]$ we are left with η_j, if this is not the case we have zero. Similarly for (5.2.17) if $\tau \in [t_{2j-1}, t_{2j}]$ we are left with ζ_j if not then we have zero. Therefore, these functions are a compact way of us implementing the complete set of η_j's and ζ_j's in two functions. The effect of such a function on our integral is

$$\int_{t_0}^{\tau} \xi(\tau)d\tau \longrightarrow \sum_{j=1}^{n} \int_{t_{2j-1}}^{\tau} d\tau \tag{5.2.18}$$

and bearing this in mind we now turn our attention back to (5.2.11)

Let us start by considering the term in (5.2.11) which is bilinear in $\xi(\tau)$,

$$exp\left\{-\frac{q_0^2}{\pi\hbar}\int_{t_0}^t d\tau \int_{t_0}^\tau ds L_2(\tau-s)\xi(\tau)\xi(s)\right\} \tag{5.2.19}$$

which using our functions (5.2.16) and (5.2.17)becomes,

$$exp\left\{-\frac{q_0^2}{\pi\hbar}\int_0^\infty J(\omega)\coth\left(\frac{\beta\hbar\omega}{2}\right)d\omega\sum_{j=1}^n\left(\int_{t_{2k}}^{t_{2j}}-\int_{t_{2k}}^{t_{2j-1}}\right)d\tau\sum_{k=1}^n\int_{t_{2k-1}}^{t_{2k}}\zeta_j\zeta_k\cos(\omega(\tau-s))ds\right\} \tag{5.2.20}$$

If we briefly consider the integrals form t_{2k} to t_{2j-1} or t_{2j} we see that for $j<k$ these integrals are clearly 0. Therefore, if we consider merely the second half of this term (5.2.20), we have

$$\sum_{k=1}^n\sum_{j\geq k}^n\int_{t_{2j-1}}^{t_{2j}}d\tau\int_{t_{2k-1}}^{t_{2k}}\zeta_j\zeta_k\cos(\omega(\tau-s))ds \tag{5.2.21}$$

which, once we evaluate these integrals, becomes

$$\frac{1}{\omega^2}\sum_{k=1}^n\sum_{j\geq k}^n\zeta_j\zeta_k[\cos(\omega(\tau_{2j}-\tau_{2k}))+\cos(\omega(\tau_{2j-1}-\tau_{2k-1}))-\cos(\omega(\tau_{2j-1}-\tau_{2k}))-\cos(\omega(\tau_{2j}-\tau_{2k-1}))] \tag{5.2.22}$$

Here for ease of notation, (as will become apparent) we change all these terms by $\cos(\omega t)\to-(1-\cos(\omega t))$ since all these 1's cancel out. This allows us to define a function,

$$Q_2(t)=\int_0^\infty\frac{J(\omega)}{\omega^2}(1-\cos(\omega t))\coth\left(\frac{\beta\hbar\omega}{2}\right)d\omega \tag{5.2.23}$$

We also consider the case $j=k$ separately. First, if $j=k$ then $\zeta_j\zeta_k=\zeta_j^2=+1$ for all j, if we also make a change of variables into $(\tau-s)$ ranging from 0 to $t_{2j}-t_{2j-1}$ for each j, we need only evaluate

$$-\int_0^{t_{2j}-t_{2j-1}}d\alpha\int_\alpha^0\cos(\omega\alpha')d\alpha'=-\frac{1}{\omega^2}[\cos(\omega(t_{2j}-t_{2j-1}))-1] \tag{5.2.24}$$

which means that the whole term bilinear in $\xi(\tau)$ in (5.2.11), once again united, becomes:

$$exp\left[-\frac{q_0^2}{\pi\hbar}\left\{\sum_{j=1}^n Q_2(t_{2j}-t_{2j-1})+\sum_{k=1}^n\sum_{j>k}^n\zeta_j\eta_k[Q_2(t_{2j-1}-t_{2k})+Q_2(t_{2j}-t_{2k-1})-Q_2(t_{2j}-t_{2k})-Q_2(t_{2j-1}-t_{2k-1})]\right\}\right] \tag{5.2.25}$$

Continuing from this we consider the other term in (5.2.11) which is of the form,

$$exp\left[\frac{iq_0^2}{\pi\hbar}\int_{t_0}^t d\tau\int_{t_0}^\tau L_1(\tau-s)\xi(\tau)\chi(s)ds\right] \tag{5.2.26}$$

As above, if $\tau<t_0$ then these integrals become zero and as such this means that in our sums j must be strictly greater than k. This noted, we write this term out as

$$exp\left[\frac{iq_0^2}{\pi\hbar}\int_0^\infty J(\omega)d\omega\sum_{k=1}^n\sum_{j>k}^n\zeta_j\eta_k\int_{t_{2j-1}}^{t_{2j}}d\tau\int_{t_{2k}}^{t_{2k+1}}\sin(\omega(\tau-s))ds\right] \tag{5.2.27}$$

motivating the definition

$$Q_1(t)=\int_0^\infty\frac{J(\omega)}{\omega^2}\sin(\omega t)d\omega \tag{5.2.28}$$

From which it is simple to show that evaluating the integrals in (5.2.27) this term can be written as

$$exp\left[\frac{iq_0^2}{\pi\hbar}\sum_{k=1}^n\sum_{j>k}^n\zeta_j\eta_k[Q_1(t_{2j}-t_{2k+1})-Q_1(t_{2j}-t_{2k})-Q_1(t_{2j-1}-t_{2k+1})+Q_1(t_{2j-1}-t_{2k})]\right] \tag{5.2.29}$$

We now need only include the factor which comes from the asymmetry of the problem

$$exp\left[-\frac{i\varepsilon}{\hbar}\int_{t_0}^t\xi(\tau)d\tau\right]=exp\left[-\frac{i\varepsilon}{\hbar}\sum_{j=1}^n\zeta_j(t_{2j}-t_{2j-1})\right] \tag{5.2.30}$$

If we now sum over all the η_k in these last two terms, as well as making the definition

$$X_{jk} = Q_1(t_{2j} - t_{2k+1}) - Q_1(t_{2j} - t_{2k}) - Q_1(t_{2j-1} - t_{2k+1}) + Q_1(t_{2j-1} - t_{2k}) \tag{5.2.31}$$

Then these last two terms become

$$\frac{1}{2}\left(exp\left[\frac{iq_0^2}{\pi\hbar}\sum_{k=1}^{n}\sum_{j>k}^{n}\zeta_j X_{jk} \right] + exp\left[-\frac{iq_0^2}{\pi\hbar}\sum_{k=1}^{n}\sum_{j>k}^{n}\zeta_j X_{jk} \right] \right) exp\left[-\frac{i\varepsilon}{\hbar}\sum_{j=1}^{n}\zeta_j(t_{2j} - t_{2j-1}) \right] \tag{5.2.32}$$

Noting that this formula is identical under sign-reversal for all the ζ_j, since we sum over $\zeta_j = \pm 1$, we write these terms as

$$2^{n-1}\Pi_{k=1}^{n}\cos\left[\frac{iq_0^2}{\pi\hbar}\sum_{j=k+1}^{n}\zeta_j X_{jk} \right]\cos\left[\sum_{j=1}^{n}\zeta_j\left[(t_{2j} - t_{2j-1})\frac{\varepsilon}{\hbar} - \frac{q_0^2}{\pi\hbar}X_{j0} \right] \right] \tag{5.2.33}$$

Finally, if we collect all these factors and make a few new definitions we finish with a set of nested equations for $P(t)$ which are ultimately defined in terms of the spectral density $J(\omega)$. Despite some repetition of previous definitions we write the complete set of equations out here for clarity and ease of reference. Our result is:

$$P(t) = \sum_{n=0}^{\infty}(-1)^n\Delta^{2n}K_n(t) \tag{5.2.34}$$

$$K_n(t) = 2^{-n}\sum_{\{\zeta_j\}}\int_0^t dt_{2n}\int_0^{t_{2n}}dt_{2n-1}...\int_0^{t_2}dt_1 F_n(\{t_m\}, \{\zeta_i\}, \varepsilon) \tag{5.2.35}$$

$$F_n(\{t_m\}, \{\zeta_i\}, \varepsilon) = F_1\{t_m\}F_2\{t_m, \zeta_i\}F_3\{t_m\zeta_i\}F_4\{t_m\zeta_i\varepsilon\} \tag{5.2.36}$$

where the four factors here labelled as F_i are given by

$$F_1 \equiv exp\left[-\frac{q_0^2}{\pi\hbar}\sum_{j=1}^{n}S_j \right] \tag{5.2.37}$$

$$F_2 \equiv exp\left[-\frac{q_0^2}{\pi\hbar}\sum_{k=1}^{n}\sum_{j=k+1}^{n}\zeta_j\zeta_k\Lambda_{jk} \right] \tag{5.2.38}$$

$$F_3 \equiv \Pi_{k=1}^{n-1}\cos\left[\frac{q_0^2}{\pi\hbar}\sum_{j=k+1}^{n}n\zeta_j X_{jk} \right] \tag{5.2.39}$$

$$F_4 \equiv \cos\left[\sum_{j=1}^{n}\zeta_j\left[(t_{2j} - t_{2j-1})\frac{\varepsilon}{\hbar} - \frac{q_0^2}{\pi\hbar}X_{j0} \right] \right] \tag{5.2.40}$$

where we have made several new definitions. The terms S_j, Λ_{jk} and X_{jk} used above are defined as

$$S_j = Q_2(t_{2j} - t_{2j-1}) \tag{5.2.41}$$

$$\Lambda_{jk} = Q_2(t_{2j-1} - t_{2k}) + Q_2(t_{2j} - t_{2k-1}) - Q_2(t_{2j} - t_{2k}) - Q_2(t_{2j-1} - t_{2k-1}) \tag{5.2.42}$$

$$X_{jk} = Q_1(t_{2j} - t_{2k+1}) - Q_1(t_{2j} - t_{2k}) - Q_1(t_{2j-1} - t_{2k+1}) + Q_1(t_{2j-1} - t_{2k}) \tag{5.2.43}$$

and we recall from earlier that Q_1 and Q_2 are defined as

$$Q_1(t) = \int_0^\infty \frac{J(\omega)}{\omega^2}\sin(\omega t)d\omega \tag{5.2.44}$$

$$Q_2(t) = \int_0^\infty \frac{J(\omega)}{\omega^2}(1 - \cos(\omega t))\coth\left(\frac{\beta\hbar\omega}{2} \right)d\omega \tag{5.2.45}$$

we immediately remark that these equations are identical to those given by Leggett et al. in [3]. Indeed I assume the derivation is identical however here much of the argument is followed while being augmented with more steps explicitly included and more discussion on certain points, especially on some of the possiblymore complex steps.

The results (5.2.34) - (5.2.45) are our key results since they essentially describe the dynamics of the spin-boson model from which many quantities of interest can be obtained. and as such will provide the foundation for the vast majority of our subsequent work. Before considering the other quantity of interest, namely $C(t)$ it will be useful and instructive to develop some more terminology and a graphical representation of paths.
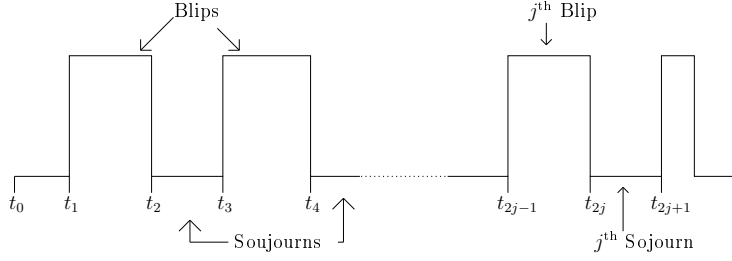
Figure 9: The standard diagrammatical representation of our four-state path where time spent in the off-diagonal elements are labelled as blips and time spent in the diagonal elements are called sojourns.

To represent a path we draw a line that runs along the x-axis whenever our system resides in a 'diagonal-state' i.e. A or D. We continue the line above and parallel when we are in a 'nondiagonal-state' B or C, see Fig.9 below,

The labels ζ_j and η_j which distinguish between states which are both diagonal or both off-diagonal respectively are evidently not included in such a diagram. We define

$$
\begin{aligned}
b_j &= t_{2j} - t_{2j-1} \\
s_j &= t_{2j+1} - t_{2j}
\end{aligned}
\tag{5.2.46}
$$

where we call b_j the 'j^{th} blip' and s_j the 'j^{th} sojourn'. That is, we will refer to the times where the line is along the x-axis and the system is in a diagonal state as sojourns, and times where it is above this line and the system is in an off-diagonal state as a blips. It is clear from the way in which we have defined them above that the jth blip precedes the jth sojourn.

Using these notations and conventions it is clear that the four components in (5.2.36) represent a variety of 'interactions' between blips and sojourns. For obvious reasons we call an interaction "repulsive" if it tends to suppress F_n and "attractive" if instead it increases it. Let us now briefly consider the four terms which constitute (5.2.36) in order that we may obtain some qualitative idea of their behaviour as well as the form of the interaction they describe.

Firstly,

$$
F_1 = exp\left[-\frac{q_0^2}{\pi\hbar} \sum_{j=1}^{n} Q_2(t_{2j} - t_{2j-1}) \right]
$$

clearly represents the interaction of a blip with itself. If we return to considering (5.2.11) and recall that F_1 comes from the term including $L_2(\tau - s)$, then when $j = k$ then $\zeta_j\zeta_k = \zeta_j^2 = 1$ and as such if we could show that the Fourier transform of $L_2(\tau - s) > 0$ then it would follow that $L_2(\tau - s)$ would be strictly repulsive. To this end we take the Fourier transform of $L_2(\tau - s)$ with respect to $(\tau - s)$,

$$
\int_{-\infty}^{\infty} e^{2\pi i(\tau-s)t} L_2(\tau - s) d(\tau - s) = \int_{-\infty}^{\infty} e^{2\pi i(\tau-s)t} \int_{0}^{\infty} d\omega J(\omega) \coth\left(\frac{\beta\hbar\omega}{2}\right) \cos(\omega(\tau - s)) d(\tau - s)
\tag{5.2.47}
$$

A reordering of the integration (which we assume is allowed as convergence properties would seem necessary for the function to make sense in the first instance), leaves us

$$
\int_{0}^{\infty} J(\omega) \coth\left(\frac{\beta\hbar\omega}{2}\right) \int_{-\infty}^{\infty} e^{2\pi i(\tau-s)t} \cos(\omega(\tau - s)) d(\tau - s) d\omega
\tag{5.2.48}
$$

where by concentrating on the second integral and express $\cos(\omega(\tau - s))$ as exponentials, we get,

$$
\frac{1}{2} \int_{-\infty}^{\infty} \left[e^{i(\tau-s)(\omega+2\pi t)} + e^{-i(\tau-s)(\omega-2\pi t)} \right] d(\tau - s) = \frac{1}{2} \left[\delta(\omega - 2\pi t) + \delta(\omega + 2\pi t) \right]
\tag{5.2.49}
$$

this then allows us to evaluate the second integral in ω. Since ω only runs from 0 to ∞ this means that only one of these δ-functions contributes at once, namely the one where $\omega = |2\pi t|$. As such we know that the Fourier transform yields

$$
f(t) = J(|2\pi t|) \coth(|\beta\hbar\pi t|) > 0
\tag{5.2.50}
$$

Thus proving our claim that F_1 is repulsive.

We next analyze,

$$
F_2 = exp\left[-\frac{q_0^2}{\pi\hbar} \sum_{k=1}^{n} \sum_{j=k+1}^{n} \zeta_j\zeta_k \Lambda_{jk} \right]
$$

51

which we can see based on the term $\zeta_j\zeta_k$ represents interactions between different blips. Although we cannot make a definite statement about the sign for this single term in the exponential, our previous argument indicates that quite generally the combination $(\sum_j S_j + \sum_{j,k} \zeta_j\zeta_k\Lambda_{jk})$ is always positive where both these sums cover the same set of blips. As such we expect that the effect of blips upon one another will be small (possibly even negligibly so) compared to the self-interaction of the blips.

The term

$$F_3 = \Pi_{k=1}^{n-1} \cos\left[\frac{q_0^2}{\pi\hbar} \sum_{j=k+1}^{n} \zeta_j X_{jk}\right] \tag{5.2.51}$$

this term "expresses the interference between processes in which the system goes, say, from A→B→A and from B→D→B: it appears as an interaction between a blip and previous sojourns only." [3] We draw a representation of the time intervals involved in the X_{jk} term, as done below in Fig.10.
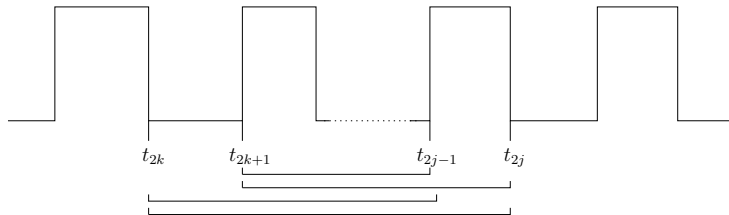

Figure 10: A representation of the four terms which constitute X_{jk}.

As we can see if $j \neq k+1$ each of these involves at least one sojourn and as such if these sojourns are very long these terms can be neglected. And so, in the limit where the $(j-1)^{\text{th}}$ sojourn tends to infinity we can reduce this to an effective self-interaction term of the form

$$\Pi_{k=1}^{n-1} \cos\left[\frac{q_0^2}{\pi\hbar} Q_1(t_{2j} - t_{2j-1})\right] \tag{5.2.52}$$

for the jth blip. We will later use this sort of argument to justify the "Non-Interacting Blip Approximation".

Finally,

$$F_4 = \cos\left[\sum_{j=1}^{n} \zeta_j\left[(t_{2j} - t_{2j-1})\frac{\varepsilon}{\hbar} - \frac{q_0^2}{\pi\hbar}X_{j0}\right]\right] \tag{5.2.53}$$

this term has a dual role, both modulating (for $\varepsilon \neq 0$) the contribution of the self-interaction of the blips as well as giving the interaction between all the blips and the zeroth sojourn. This term is not particularly important in the unbiased case, however for finite bias of $\varepsilon \neq 0$, it is essential to keep. This can readily be seen from the fact that it is the only term which depends on whether we start in the upper or lower well. We would expect that for large t, $P(t)$ will behave qualitatively differently in the two cases.

We now turn our attention to the study of the quantity $C(t)$ defined earlier. We do not exhaustively derive equations analogous to those we obtained for $P(t)$, however we do qualitatively consider the behaviour of this quantity.

5.3 Expression for $C(t)$

We now briefly indicate a manner in which we may derive an analogous expression to (5.2.34) for the symmetrized correlation function which we defined earlier as

$$C(t) = \frac{1}{2}\langle\{\hat{\sigma}_z(t), \hat{\sigma}_z(0)\}\rangle_\beta \equiv \frac{1}{2Z}Tr[\hat{\sigma}_z(t)\hat{\sigma}_z(0) + \hat{\sigma}_z(0)\hat{\sigma}_z(t)] \tag{5.3.1}$$

where Z denotes the partition function and with $\sigma_z(t)$ being considered in the Heisenberg representation in terms of the full Hamiltonian $\hat{H}$ is

$$\sigma_z(t) \equiv e^{\frac{i\hat{H}t}{\hbar}}\hat{\sigma}_z e^{-\frac{i\hat{H}t}{\hbar}} \tag{5.3.2}$$

We begin by considering a different quantity $P(\sigma', \sigma : t)$, which we call the joint probabilities. Suppose at t=0 the system environment composite is in thermal equilibrium (equivalent to requiring a density matrix proportional to $e^{-\beta\hat{H}}$). At our initial time we observe our system to have a value $\sigma = \pm 1$ of $\hat{\sigma}_z(t)$, with the system not being disturbed by this observation. Then if the system is later observed at a time t and found to have value σ' the probability for this sequence is defined to be $P(\sigma', \sigma : t)$. We now want to relate this to our quantity of interest $C(t)$, and to this end we define projection operators,

$$\hat{\pi}_\pm \equiv \frac{1}{2}(1 \pm \hat{\sigma}_z) \tag{5.3.3}$$

We use these now, when we consider the quantity defined by

$$\sum_{\sigma'} \sigma' P(\sigma', \pm 1 : t) \tag{5.3.4}$$

which we can trivially express as

$$\frac{1}{4} < \hat{\sigma}_z(t) \pm \hat{\sigma}_z \hat{\sigma}_z(t) \pm \hat{\sigma}_z(t)\hat{\sigma}_z + \hat{\sigma}_z \hat{\sigma}_z(t)\hat{\sigma}_z >_\beta \tag{5.3.5}$$

where $\hat{\sigma}_z$ represents our initial value ± 1. We now use the trace rule developed in Ch.2 and note that the density matrix is of the form $e^{-\beta \hat{H}}/Z$. This gives

$$Tr\left\{ (\hat{\sigma}_z(t) \pm \hat{\sigma}_z \hat{\sigma}_z(t) \pm \hat{\sigma}_z(t)\hat{\sigma}_z + \hat{\sigma}_z \hat{\sigma}_z(t)\hat{\sigma}_z)e^{-\beta \hat{H}} \right\} /Z \tag{5.3.6}$$

and thus by finally expressing these σ's in terms of our projection operators $\hat{\pi}_\pm$ defined above we are left with

$$\sum_{\sigma'} \sigma' P(\sigma', \pm 1 : t) = < \hat{\pi}_\pm \hat{\sigma}_z(t)\hat{\pi}_\pm >_\beta \tag{5.3.7}$$

If we now continue by writing,

$$-\sum_{\sigma'} \sigma' P(\sigma', -1 : t) + \sum_{\sigma'} \sigma' P(\sigma', +1 : t) = \sum_{\sigma \sigma'} \sigma \sigma' P(\sigma', \sigma : t) \tag{5.3.8}$$

then we get,

$$\sum_{\sigma \sigma'} \sigma \sigma' P(\sigma', \sigma : t) = < \hat{\pi}_+ \hat{\sigma}_z(t)\hat{\pi}_+ >_\beta - < \hat{\pi}_- \hat{\sigma}_z(t)\hat{\pi}_- >_\beta = \frac{1}{2} < \hat{\sigma}_z(t)\hat{\sigma}_z(0) + \hat{\sigma}_z(0)\hat{\sigma}_z(t) >_\beta \tag{5.3.9}$$

Which gives us the intuitively rather obvious result that

$$C(t) = \sum_{\sigma \sigma'} \sigma \sigma' P(\sigma', \sigma : t) \tag{5.3.10}$$

For simplicity we shall limit our considerations hereafter to the unbiased case of $\varepsilon = 0$, the generalization is not particularly taxing. In this case, the symmetry implies that $C(t)$ reduces simply to the expectation value of $\hat{\sigma}_z$ at time t, and given that at time t=0 we are in the state $\hat{\sigma}_z = \pm 1$. However such a prescription is not necessarily identical to the $P(t)$ for which we derived exact equations for, since it has an arbitrary combination of blips and sojourns prior to t=0. However this demonstrates that both $C(t)$ and $P(t)$ are limit values of a more general quantity $P(t_c; t)$ defined as the expectation value of $\hat{\sigma}_z$ at time $t > 0$ where we allow the system to change states only before t_c. In this notation the limit $t_c \to 0$ represents $C(t)$ and the limit $t_c \to \infty$ represents $P(t)$.

We finally briefly note that the effect of this change is generally not simply to multiply the series for $P(t)$ by another power series due to the interaction between blips and sojourns before t=0 and those after. However in the approximation we now outline called the 'Non-Interacting Blip Approximation', it is clear that $P(t)$ and $C(t)$ are negligibly different.

5.4 The Non Interacting-Blip Approximation

Equations (5.2.34) - (5.2.45) are, while exact, extremely cumbersome and awkward to use practically. We here outline an approximation which simplifies these equations enormously and also turns out to be exact in certain regions of the parameter space up to lowest order of $\frac{\Delta}{\omega_c}$, as well as being very close in most of the remaining parameter space. This approximation consists of two parts:

1. All factors of X_{jk} in (5.2.39) and (5.2.40) are set to zero except for $k = j - 1$ which we change so that $X_{j,j-1} = Q_1(t_{2j} - t_{2j-1})$.

2. Enforce $\Lambda_{jk} \equiv 0$ in equation (5.2.38).

We motivate these prescriptions in more detail in the next chapter for the particular case of ohmic dissipation ($J(\omega) \sim \omega$). However, we make some effort at demonstrating that such simplifications are at least reasonable. A more detailed analysis can be found in Sect IV.C of [3], from which much of the analysis below is based upon.

Let us begin by considering the first approximation and state that it will be misleading in two cases:

1. If there are strong cancellations in the multiple integrals of (5.2.35) such that terms of order $\left(\frac{\Delta}{\omega_c}\right)^L$ ($L > 0$) become important.

2. If terms of order $\left(\frac{\Delta}{\omega_c}\right)^L$ "add up" in the series (5.2.34) so as to become important for large t. However the timescale we expect this to occur on makes it fall outside of our range of "interesting times".

We also note here that if the integrand of Eq.(5.2.35) is positive definite (as it is for the ohmic case with $\alpha < \frac{1}{2}$), then the first case has no chance of occurring. Indeed for $\varepsilon = 0$ it seems very likely that this simplification is valid for our purposes and for $\varepsilon \neq 0$ the only likely exception is in the ohmic case and the region $\frac{1}{2} < \alpha < 1$, which we will not consider in detail during this report.

The justification for the second approximation is more cumbersome. We naturally see that this approximation should hold iff the length of a typical sojourn is sufficiently large and $Q_2(t)$ falls off at a rate great enough that all the Q_2's $\ll 1$ for $j \neq k$. However, for ohmic ($J(\omega) \sim \omega$) and subohmic ($J(\omega) \sim \omega^s$) ($s < 1$), Q_2 increases with t and as such this does not hold in the general case. Given this, we consider the so-called "Golden-rule" limit.

If the function $Q_2(t)$ increases with t, then the factor F_1 (5.2.37) will suppress long blips to such an extent that a typical blip is very short in comparison to a typical sojourn. If we thus consider Fig.11 below it is clear that the all the terms in Λ_{jk} are all approximately equal and as such $\Lambda_{jk} \approx 0$. As mentioned before, this approximation will be more rigorously demonstrated when we consider the ohmic case in the next chapter.
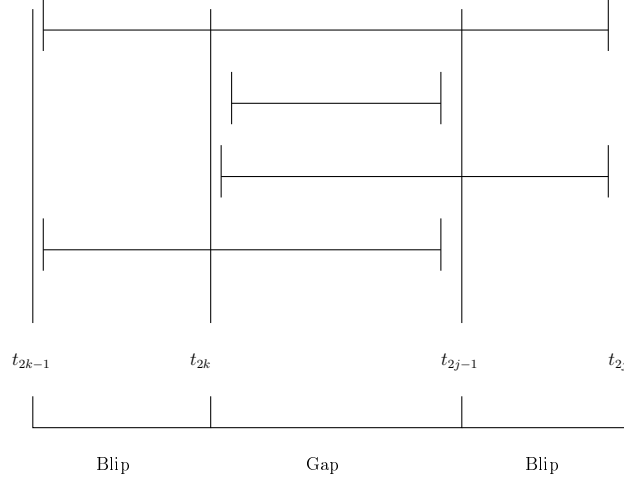

Figure 11: A representation of the four terms in Λ_{jk} which constitute Q_2 in (A.3.36). The section labelled 'gap' necessarily contains at least one blip-sojourn pair for $j \neq k$

It is obvious that use of this approximation drastically reduces the complexity of our equations and as such the problem of finding $P(t)$. Let us now consider the unbiased case of $\varepsilon = 0$ which reduced F_4 (Eq.(5.2.40)) and as such is a particularly simple case. With these provisos made then Equation (5.2.36), reduces to

$$F_n(\{t_i\}) = \Pi_{j=1}^n \cos\left[\frac{q_0^2}{\pi\hbar} Q_1(t_{2j} - t_{2j-1})\right] exp\left[-\frac{q_0^2}{\pi\hbar} Q_2(t_{2j} - t_{2j-1})\right] \tag{5.4.1}$$

which gives us an expression for $P(t)$ as

$$P(t) = \sum_{n=0}^{\infty} \int_0^t dt_{2n} \int_0^{t_{2n}} dt_{2n-1}... \int_0^{t_2} dt_1 \Pi_{j=1}^n f(t_{2j} - t_{2j-1}) \tag{5.4.2}$$

where we have defined the function $f(t)$ as,

$$f(t) = \Delta^2 \cos\left[\left(\frac{q_0^2}{\pi\hbar}\right) Q_1(t)\right] exp\left[-\frac{q_0^2}{\pi\hbar} Q_2(t)\right] \tag{5.4.3}$$

The formal similarity between Eq.(5.4.2) and the partition function we would obtain based on a system of particles which are in a one-dimensional fixed volume leads us to make the following change. We switch to an isobaric ensemble through a Laplace transform

$$\tilde{P}(\lambda) = \int_0^\infty e^{-\lambda t} P(t) dt \tag{5.4.4}$$

A few changes in the integration variables and order of integration yields,

$$\tilde{P}(\lambda) = \sum_{n=0}^{\infty} (-1)^n \int_0^\infty dt \int_0^\infty dt_1... \int_0^\infty dt_{2n} e^{-\lambda(t_1+t_2+...+t_{2n})} \Pi_{j=1}^n f(t_{2j})$$

$$= \sum_{n=0}^{\infty} (-1)^n \left[f(\lambda)\right]^n / \lambda^{n+1} = \left[\lambda + f(\lambda)\right]^{-1} \tag{5.4.5}$$

54

where $f(\lambda)$ is the Laplacian transform of $f(t)$ and as such is defined as

$$f(\lambda) = \Delta^2 \int_0^\infty \cos\left[\frac{q_0^2}{\pi\hbar}Q_1(t)\right] exp\left[-(\lambda t + \frac{q_0^2}{\pi\hbar}Q_2(t))\right] dt \tag{5.4.6}$$

Given this it seems, in principle, that $f(\lambda)$ should be calculable for any form of $J(\omega)$. Such a transform can then be inverted to obtain $P(t)$,

$$P(t) = \frac{1}{2\pi i}\int_C e^{\lambda t}\tilde{P}(\lambda)d\lambda \equiv \frac{1}{2\pi i}\int_C e^{\lambda t}\left[\lambda + f(\lambda)\right]^{-1}d\lambda \tag{5.4.7}$$

where C is the standard Bromwich contour. Even when explicit inversion is troublesome, much can be learned from a study of $\tilde{P}(\lambda)$.

As such Equation (5.4.7) with the definitions (5.4.6), (5.2.44) and (5.2.45) supplies a complete solution to the dynamics of the unbiased spin-boson model within our approximation. We also make the observation that $C(t)$ and $P(t)$ are identical in this approximation for $\omega_c t \ll 1$, since by this time there is no interaction between positive- and negative-time parts of the path. However this is not strictly rigorous, merely since interblip interactions are negligible in the calculation of $P(t)$ does not necessarily mean the same holds true for $C(t)$ although it would be extremely bizarre if such interactions had a dramatic effect.

This means we have found a simplified expression for the dynamics of the Spin-Boson model in terms of the spectral density function $J(\omega)$. In obtaining this expression we have relaxed the Markov assumption of the previous chapter to a pseudo-Markovian assumption namely, the Non-Interacting Blip approximation. We will now take a specific form for the spectral density and analyze the dyanmics for the exact solution in order that we might justify the Non-Interacting Blip approximation for this choice of Spectral Density function. it is clear that provided the approximation is justified the equations for $P(t)$ are both more precise and arguably simpler to analyze thn the Born-Markov master-equation of last chapter. We will not however have chance to explicitly compare the dynamics between this equation and the master-equation results but suffice to say that the above results are much more useful in our regimes of interest in finding quantities of interest such as the timescale of decoherence and dissipation. Before we proceed however we will briefly summarise the most salient points of the above chapter

5.5 Summary

- We firstly gave a (non-rigorous) justification for the Hamiltonian we used in the Spin-Boson model, while noting that [3] justified this Hamiltonian from purely physical considerations.

- We made several remarks for the domain on which our model will be valid based on the physical considerations of [3], namely: $\frac{\Delta}{\omega_c}$, $\frac{kT}{\hbar\omega_c}$ and $\frac{\varepsilon}{\hbar\omega_c} \ll 1$.

- We gave the spectral density function a general power law form and brieflyconsidered some of the differences between different powers, with specific reference to the dimensionless dissipation coefficient α in the ohmic case.

- We defined two quantities of interest $P(t)$ the expectation value (under specific initial conditions) and $C(t)$ the symmetrized equilibrium correlation function.

- We used work done y Legget et. al. [3], iteself taken in places from the work of Feynman to transform our problem for $P(t)$ into one of evaluating the influence functional and in turn a 4-state path integral.

- We solved for $P(t)$ in terms of an infinite sum of mutually exclusive integrals and proceeded to give a short interpretation of each of the terms inside the integrals.

- We briefly demonstrated that similar work could be carried out to find a power series for $C(t)$, but that this quantity should not be drastically different from $P(t)$ for t large enough.

- We discussed the implementation of an approximation called the Non-Interacting Blip approximation and gave a vague idea of justifying this approximation for general $J(\omega)$, however a more rigorous justification will be givwen next chapter for the specific form of the spectral density function which we choose.

- We imposed the approximation on our general solution and reduced it to a much more manageable form, from which it would be possible to study the dynamics of the modelin certain regimes of the parameters T - Temperature and α - Dissipation.

6 Ohmic Dissipation in the Spin-Boson Model

In this chapter we apply the results of the previous section to the specific example of ohmic dissipation ($J(\omega) \sim \omega$ for $\omega \lesssim \omega_c$) and thereby gain an expression for $P(t)$ in the Non-Interacting Blip approximation. This chapter will be structured much as Section V. of [3], in that we will consider several extreme regions of the (α, T)-phase space individually and having justified the approximation in these regions we motivate its wider application.

We begin by giving a specific form for our spectral density, namely

$$J(\omega) = \eta\omega exp^{-\frac{\omega}{\omega_c}} \tag{6.0.1}$$

with ω_c being an arbitrary high-frequency cut-off as described before. We also define a dimensionless dissipation coefficient α,

$$\alpha \equiv \frac{\eta q_0^2}{2\pi\hbar} \tag{6.0.2}$$

We consider the case where the "bare tunneling amplitude" Δ and the cut-off ω_c are such that $\frac{\Delta}{\omega_c} \ll 1$ as well as being in the time regime $\omega_c^{-1} \ll t$, alongside the requirement that t is sufficiently small, such that $P(t)$ is not negligibly small itself in the unbiased case, or settled into one state in the biased case. We will refer to such a time regime throughout as "interesting times". Given this our problem becomes describing the behaviour of $P(t)$ as a function of the temperature T and the dimensionless coefficient α.

At this point we briefly remark that the quantity Δ is proportional to ω_c^α. It is evident that we would want any result to be independent of the arbitrarily chosen high-frequency cut-off. As such we expect our results to be given with respect to the variable,

$$\Delta_r \equiv \Delta \left[\frac{\Delta}{\omega_c}\right]^{\frac{\alpha}{1-\alpha}} \tag{6.0.3}$$

which can be easily verified as being independent of ω_c. Were we to encounter regions of phase-space where Δ and ω_c are not in this combination, then these regions may well be sensitive to details which we have not considered.

6.1 General Formulae

In Appendix A we put the above form for the spectral density function into our previously derived exact equations from the last chapter. The details of the derivation are to be found in the appendix where it is demonstrated that without using approximations on top of our already established regimes of interest, we reach this set of equations, which we now state together for ease of reference.

$$F_1 = \prod_{j=1}^{n} \left[f'(b_j)\right]^{2\alpha} \tag{6.1.1}$$

$$F_2 = \prod_{k=1}^{n-1} \prod_{j=k+1}^{n} \left[\frac{f'(u_{jk} + b_j + b_k)f'(u_{jk})}{f'(u_{jk} + b_j)f'(u_{jk} + b_k)}\right]^{2\alpha\zeta_j\zeta_k} \tag{6.1.2}$$

$$F_3 = \prod_{k=0}^{n-1} \cos\left[2\alpha \sum_{j=k+1}^{n} \tan^{-1}\left(\frac{b_j s_k(b_j + s_k + 2y_{jk})}{s_k^2 + (1 + y_{jk}(y_{jk} + s_k))(1 + (y_{jk} + b_j)(y_{jk} + b_j + s_k))}\right)\zeta_j\right] \tag{6.1.3}$$

$$f'(t) = (1 + t^2)^{-\frac{1}{2}}\left(\frac{\beta\hbar\omega_c}{\pi t}\sinh\left(\frac{\pi t}{\beta\hbar\omega_c}\right)\right)^{-1} \tag{6.1.4}$$

We finally note that there is an alternative set of influence functions (F_n), which avoid the explicit cosine function and which are therefore useful. We give these functions as well, since we will later occasionally use them. However, we will not derive the expressions explicitly, (they are taken from [3]) rather we simply state them.

$$F_n\{t_i, \zeta_i : 0\} = 2^{-n} \sum_{\eta_j=\pm 1} \left[\Phi\{t_i, \zeta_i, \eta_i\}\right]^{2\alpha} \tag{6.1.5}$$

$$\Phi\{t_i, \zeta_i, \eta_i\} \equiv \prod_{j=1}^{n} \frac{g(b_j)}{(1 + b_j^2)}\left[1 + y_{j0}(y_{j0} + b_j) + i\eta_0\zeta_1\zeta_j b_j\right]\prod_{k=1}^{j-1}\left[(D_{jk} + i\eta_k\zeta_j\zeta_{k+1}E_{jk})G_{jk}^{(\zeta)}M_{jk}^{(\zeta)}\right] \tag{6.1.6}$$

$$D_{jk} \equiv [1 + y_{jk}(y_{jk} + s_k)][1 + (y_{jk} + b_j)(y_{jk} + b_j + s_k)] + s_k^2 \tag{6.1.7}$$

$$E_{jk} \equiv b_j s_k(b_j + s_k + 2y_{jk}) \tag{6.1.8}$$

$$M_{jk}^{(\zeta)} \equiv \left[\frac{g(y_{jk} + b_j + b_k + s_k)g(y_{jk} + s_k)}{g(y_{jk} + b_j + s_k)g(y_{jk} + b_k + s_k)}\right]^{\zeta_j\zeta_k} \tag{6.1.9}$$

$$G_{jk}^{(\zeta)} = \left\{ \left[1 + (y_{jk} + s_k)^2 \right] \left[1 + (y_{jk} + b_j + b_k + s_k)^2 \right] \right\}^{-1} \qquad \text{if} \qquad \zeta_j = \zeta_k$$

$$= \left\{ \left[1 + (y_{jk} + b_j + s_k)^2 \right] \left[1 + (y_{jk} + b_k + s_k)^2 \right] \right\}^{-1} \qquad \text{if} \qquad \zeta_j = -\zeta_k \qquad (6.1.10)$$

$$g(t) = \frac{\pi t}{\beta \hbar \omega_c} \text{cosech} \left(\frac{\pi t}{\beta \hbar \omega_c} \right) \qquad (6.1.11)$$

6.2 The Line $\alpha = \frac{1}{2}$

In the second subsection of Appendix A, we justify the following equation without explicitly implementing the Non-Interacting Blip approximation,

$$F_n \{t_i\} = \prod_{j=1}^{n} \left[\frac{1}{1 + b_j^2} \right] \qquad (6.2.1)$$

which is precisely the result which would have been attained if we had simply made the Non-Interacting Blip approximation from the outset. What the work in the Appendix has done is demonstrate that the relative corrections to each of the $K_n(t)$ neglected in this approximation is rigorously of order at most $t^{-1}(ln(t))^2$. Which ultimately allows us reach the equation

$$K_n(t) = \left(\frac{\pi}{2} \right)^n \frac{(\omega_c t)^n}{n!} \left[1 + O((\omega_c t)^{-1} (\ln(\omega_c t))^2) \right] \qquad (6.2.2)$$

As such through neglecting any correction terms, then the series for $P(t)$ can be trivially summed and yields the result

We briefly remark that the above result is not "exact" in the limit $\omega_c \to \infty$. This is because it does not follow directly that since corrections to each $K_n(t)$ are at most of order $(\omega_c t)^{-1}(\ln(\omega_c t))^2$ in the limit $t \to \infty$, that the corrections to the oscillating series $P(t)$ are of equivalent order. The most we are able to rigorously demonstrate is that such corrections are negligible up to a point, whereby the value for $P(t)$ has fallen to be of order $\left(\frac{\Delta}{\omega_c} \right)$.

$$P(t) = \sum_{n=0}^{\infty} (-1)^n \Delta^{2n} K_n(t) = 1 - \frac{\pi}{2} \omega_c t \Delta^2 + \left(\frac{\pi}{2} \omega_c t \Delta^2 \right)^2 2! \pm \dots$$

$$= exp \left[-\frac{\pi}{2} \omega_c t \Delta^2 \right] \qquad (6.2.3)$$

It is simple to show that the introduction of a non-zero finite temperature does no alter our argument, provided we maintain $\beta \hbar \omega_c \gg 1$. The only difference which we have comes from the multiplication by two more terms, namely $g(b_j)$ being a single-blip term and $M_{jk}^{(\zeta)}$ being a class of interblip interactions. Since we have the function,

$$\frac{\sinh(x + a + b) \sinh(x)}{\sinh(x + a) \sinh(x + b)} \qquad (6.2.4)$$

We can bound this below by $\frac{(x+a+b)(x)}{(x+a)(x+b)}$ simply through a Taylor series expansion of $\sinh(x) = x + \frac{x^3}{3!} + \frac{x^5}{5!} + \dots \geq x$, $\forall x \geq 0$. We can then use the exponential representation of the sinh function to obtain an upper bound of unity

$$\frac{(e^{x+a+b} - e^{-(x+a+b)})(e^x - e^{-x})}{(e^{x+a} - e^{-(x+a)})(e^{x+b} - e^{-(x+b)})} \qquad (6.2.5)$$

which can be rearranged to get

$$\frac{\cosh(2x + a + b) - \cosh(a + b)}{\cosh(2x + a + b) - \cosh(a - b)} \leq 1 \qquad (6.2.6)$$

where the inequality holds since $x, a, b \geq 0$. Hence it is clear that the factor $M_{jk}^{(\zeta)}$ lies between unity and

$$\left[\frac{(y_{jk} + b_j + s_k)(y_{jk} + b_k + s_k)}{(y_{jk} + b_j + b_k + s_k)(y_{jk} + s_k)} \right]^{\zeta_j \zeta_k} \qquad (6.2.7)$$

and evidently does not affect the argument in the Appendix regarding the powers of the b_j's and s_j's. Indeed, in the case of very large s_j's we can take this factor as unity. This leaves us with the sole effect of finite non-zero temperature for large t being to multiply every factor $(1 + b_j^2)^{-1}$ by $g(b_j)$. If we consider the integral

$$\int_0^{\infty} g(b_j : T)(1 + b_j^2)^{-1} db_j \qquad (6.2.8)$$

where

$$g(b_j : T) = \frac{\pi b_j}{\beta \hbar \omega_c} \text{cosech} \left(\frac{\pi b_j}{\beta \hbar \omega_c} \right) \qquad (6.2.9)$$

then we see that provided we have $\beta\hbar\omega_c \gg 1$, then $g(b_j : T) \sim 1$, allowing our integral to be once more temperature independent. Therefore, equation (6.2.3) holds along the line $\alpha = \frac{1}{2}$ in the (α, T)-plane for all finite temperatures.

We do not, for reasons of space, derive analogous values for the Born-Markov master-equation and compare the two, although this would be a very interesting and instructive comparison. Instead we simply make a few observations for what we expect the results to be in such a case and what we could conclude from the comparison. Firstly, this region would be particularly interesting in a comparison, since it is less affected by temperature meaning that other factors will be more susceptible to analysis without temperature effects clouding there role. More generally, since the Non-Interacting Blip approximation is 'exact', we expect fairly good qualitative agreement between the Born-Markov master-equation and these results for most temperatures, although for extreme temperatures we expect divergence unless the Born-Markov master-equation also emerges approximately independent of temperature, this would indicate that the Markov approximation is innappropriate in such regions. Alternatively, if the Born-Markov method leads to strong matching for all temperatures, then it would strongly indicate that the Born-Markov equations are a very good approximation. Finally we remark that from these results, it becomes apparent that all we need to discover a relaxation rate is the two values Δ and ω_c, both of which are experimentally accesible quantities.

6.3   High temperatures and/or Strong Dissipation

The approach followed here and in the Appendix which is implicitly used in some of the following subsections, is founded on the observation that the blip-sojourn pairs which contribute appreciably to $K_n(t)$ have length of order $\frac{t}{n}$. This is as a result from the lack of any factor to suppress sojourns in the same way F_1 suppresses blips. As we see from (6.1.1), F_1 is independent of the sojourns and F_2 and F_3, as shown previously for the specific case of $\alpha = \frac{1}{2}$, tend to constant values in the limit $s_k \to \infty$ for fixed finite b_j.

Thus it follows on phase-space grounds alone that the dominant contribution will be from lengths of order $\frac{t}{n}$. This argument could feasibly fail if for some reason, such as near-exact cancellations, the contribution of such pairs were "anomalously small" ([3] SecV.C). However in appendix D.1 of [3] this possibility is excluded rigorously for $\alpha < \frac{1}{2}$, $T = 0$ and the paper postulates that it only seems to occur in the regime $T \to 0$, $\frac{1}{2} < \alpha < 1$ which we shall consider later.

We continue by imposing our requirement of "interesting times" on $P(t)$ such that it is not negligibly small. If for example, we found that $P(t)$ had the form of an exponential decay $P(t) \sim e^{-\frac{t}{\tau}}$, then in a series for $P(t)$ the nth term becomes important roughly when $t \sim n\tau$. Which by our earlier discussion means that the characteristic length of a blip-sojourn pair is of order τ. To extend this to a more general setting we remark that the length will be of the order of the shortest characteristic timescale associated to the series expression $P(t)$ other than ω_c^{-1}. This time can be calculated provided it is done self-consistently under all our assumptions.

If we consider the factor F_1 in the influence function, all blips with a length $b_j \gg \frac{\beta\hbar}{\alpha}$ contribute an exponentially small amount, since

$$\left[f'(b_j)\right]^{2\alpha} = \left[\frac{\left(\frac{\pi t}{\beta\hbar\omega_c}\right)\operatorname{cosech}\left(\frac{\pi t}{\beta\hbar\omega_c}\right)}{(1+t^2)^{\frac{1}{2}}}\right]^{2\alpha} \tag{6.3.1}$$

where $\operatorname{cosech}(x) \sim e^{-x}$ for $x \gg 1$, therefore $\left[f'(t)\right]^{2\alpha} \sim e^{-\frac{2\pi t\alpha}{\beta\hbar\omega_c}}$ from which our claim follows. It is easy to verify that the other factors cannot cancel this small factor. Therefore, if $\frac{\beta\hbar\omega_c}{2\pi\alpha}$ is much less than the typical timescale defined earlier, it seems legitimate in evaluating $K_n(t)$ to take all blip lengths to be negligibly short compared to the length of a sojourn. This allows us to simplify our formulae enormously.

$$F_2 = \left[\frac{f'(b_j + b_k + u_{jk})f'(u_{jk})}{f'(b_j + u_{jk})f'(b_k + u_{jk})}\right]^{2\alpha\zeta_j\zeta_k} \longrightarrow \left[\frac{f'(u_{jk})f'(u_{jk})}{f'(u_{jk})f'(u_{jk})}\right]^{2\alpha\zeta_j\zeta_k} = 1 \tag{6.3.2}$$

and

$$X_{jk} = \tan^{-1}\left[\frac{b_j s_k(b_j + s_k + 2y_{jk})}{[1 + y_{jk}(y_{jk} + s_k)][1 + (y_{jk} + b_j)(y_{jk} + b_j + s_k)] + s_k^2}\right] \simeq \tan^{-1}(0) = 0 \tag{6.3.3}$$

leaving $F_3 \simeq 1$. Therefore the influence function reduces to the simple form

$$F_n\{t_i, \zeta_i : 0\} = \prod_{j=1}^{n} \cos[2\alpha\tan^{-1}(\omega_c b_j)]\left[\left(\frac{\pi b_j}{\beta\hbar}\right)\frac{\operatorname{cosech}\left(\frac{\pi b_j}{\beta\hbar}\right)}{(1 + (\omega_c b_j)^2)^{\frac{1}{2}}}\right]^{2\alpha} \tag{6.3.4}$$

which is (as anticipated), the result we would have expected since it is what we would have obtained merely by making the Non-interacting Blip approximation from scratch. We can add to this the observation that as a result of our earlier claims, the length of a blip is strongly suppressed by the factor $f(b_j)$, we can extend the limit of integration to infinity when integrating over b_j. Each blip-sojourn pair (b_j, s_j) contributes a factor proportional to $t_{2j} - t_{2j-2}$, which, using the mutual exclusion of the pairs leaves us with a simple exponential formula.

It is possible to verify that we can evaluate (see Ch.3 of [3])

$$\int_0^\infty f'(t;\alpha;\beta)dt = F(\alpha,\beta) = \frac{\sqrt{\pi}}{2}\frac{\Gamma(\alpha)}{\Gamma(\alpha+\frac{1}{2})}\left[\frac{\pi k_\beta T}{\hbar\omega_c}\right]^{2\alpha-1} \tag{6.3.5}$$

which leaves us (noting the factor of $(-1)^n$ from changing integral variables):

$$= \sum_n \int_0^t d(b_n+s_n)\int_0^{(b_n+s_n)} d(b_{n-1}+s_{n-1})...\int_0^{(b_1+s_1)} F(\alpha,\beta)^n\frac{\Delta^{2n}}{\omega_c^n}(-1)^n d\alpha$$

$$= \sum_n \left(\frac{t\, F(\alpha,\beta)\Delta^2}{\omega_c}\right)^n\frac{(-1)^n}{n!} = e^{-\frac{t}{\tau}} \tag{6.3.6}$$

where we have made the definition,

$$\tau^{-1} = \left(\frac{\Delta^2}{\omega_c}\right)F(\alpha,\beta) \tag{6.3.7}$$

This is analogous to what is referred to as the "golden rule" result (Sec III.D [3]) in the case of ohmic dissipation.

Let us briefly consider our renormalized tunneling frequency Δ_r defined earlier. We note

$$\frac{\Delta^2}{\omega_c^{2\alpha}} = \left(\frac{\Delta^{\frac{2}{2-2\alpha}}}{\omega_c^{\frac{2\alpha}{2-2\alpha}}}\right)^{(2-2\alpha)} = \left(\frac{\Delta^{\frac{2-2\alpha+2\alpha}{2-2\alpha}}}{\omega_c^{\frac{2\alpha}{2-2\alpha}}}\right)^{(2-2\alpha)} = \left(\Delta\left(\frac{\Delta}{\omega_c}\right)^{\frac{\alpha}{1-\alpha}}\right)^{(2-2\alpha)} \tag{6.3.8}$$

leaving $\Delta_r^{(2-2\alpha)}$, allowing us to rewrite τ^{-1} as

$$\tau^{-1} = \frac{1}{2\sqrt{\pi}}\frac{\Gamma(\alpha)}{\Gamma(\alpha+\frac{1}{2})}\frac{\Delta_r^2}{k_\beta T/\hbar}\left[\frac{\pi k_\beta T}{\hbar\Delta_r}\right]^{2\alpha} \tag{6.3.9}$$

We thus see, τ depends only on Δ_r as we earlier forecast and, importantly, is independent of ω_c.

Let us now concern ourselves with the "self-consistency" of the procedure by which we obtained these results. The basic tenet was that the blips had a characteristic length of $\frac{\beta\hbar}{\alpha}$, which was much smaller than the characteristic time (other than ω_c^{-1}) defined in our series for $P(t)$, therefore we require $\frac{\beta\hbar}{\alpha} \ll \tau$ as defined above. Meaning

$$\frac{\beta\hbar}{\alpha} \ll \left[\frac{\Delta^2}{\omega_c}\frac{\sqrt{\pi}}{2}\frac{\Gamma(\alpha)}{\Gamma(\alpha+\frac{1}{2})}\left[\frac{\pi k_\beta T}{\hbar\omega_c}\right]^{2\alpha-1}\right]^{-1} \tag{6.3.10}$$

which, by getting rid of coefficients on the order of unity and rearranging, we can rewrite as

$$\frac{\alpha}{\beta\hbar} \gg \left[\frac{\Delta^2}{\omega_c^{2\alpha}}\frac{\Gamma(\alpha)}{\Gamma(\alpha+\frac{1}{2})}\left[\frac{k_\beta T}{\hbar}\right]^{2\alpha-1}\right] \tag{6.3.11}$$

which, since $\beta\hbar > 0$, we can write as

$$\frac{\alpha}{(\beta\hbar)^{(2-2\alpha)}} \gg \Delta_r^{(2-2\alpha)}\frac{\Gamma(\alpha)}{\Gamma(\alpha+\frac{1}{2})} \Rightarrow (\beta\hbar)^{-1} \gg \Delta_r^{-1}\left(\frac{\Gamma(\alpha)}{\Gamma(\alpha+\frac{1}{2})}\right)^{\left(\frac{1}{2-2\alpha}\right)} \tag{6.3.12}$$

For $\alpha \ll 1$ we approximate $\Gamma(\alpha) \sim \alpha^{-1}$ and $\Gamma(\alpha+\frac{1}{2}) \sim \Gamma(\frac{1}{2})$ which we ignore since it is of order unity, giving us

$$\frac{k_B T}{\hbar} \gg \Delta_r\alpha^{\left(\frac{\alpha}{1-\alpha}\right)} \simeq \Delta_r\alpha \tag{6.3.13}$$

However for larger values of α the dependence of the quantity in brackets in (6.3.12), is relatively weak barring when $\alpha \simeq 1$. Thus we can, generally speaking, impose the condition as

$$\frac{\alpha k_B T}{\hbar} \gg \Delta_r \tag{6.3.14}$$

However such a condition is too stringent near $\alpha = 1$. For $\alpha > 1$, given that by hypothesis Δ and $\frac{k_\beta T}{\hbar} \ll \omega_c$, the criterion is automatically fulfilled for any temperature. Therefore, our result should hold for all $\alpha > 1$, which matches (apart from prefactors) the results of Bray and Moore (1982) [1]. We finally remark that this is valid for vast portions of the phase-space to the left of $\alpha = 1$, despite the radically different physics in the two extremes. We made the assumption in the Born-Markov case of weak-interaction, so the fact we have exact solutions for this region in the Non-interacting Blip approximation demonstrates the superiority of our new work, since it is very unlikely that we have even qualitative matching in this region with the Born-Markov results.

6.4 T=0 , $0 \le \alpha < \frac{1}{2}$.

We next consider that region of phase space where temperature is zero and our dimensionless dissipation coefficient α lies between zero and a half. We expect on rather general grounds that the weaker the interaction between system and environment, the more likely the evolution will display the oscillations analogous to an isolated system. As we should expect that interaction strength grows with α and T, this region seems (in an ohmically dissipative setting) the most promising for observing oscillations. As such were we to consider so-called macroscopic quantum coherence phenomena (such as in [2]), it is this region of phase space which is of most interest.

As earlier we include F_4 within F_3, and let us imagine that we could legitimately set $F_3 = F_4 = 1$. In this case the expression for $K_n(t)$ simplifies to a multiple integral given by

$$\int_0^\infty dt_{2n} \int_0^{t_{2n-1}} ... \int_0^{t_2} dt_1 \prod_{j=1}^n \left[1 + \omega_c^2(t_{2j} - t_{2j-1})^2\right]^{-\alpha} \tag{6.4.1}$$

In our regime of $\alpha < \frac{1}{2}$ and $\omega_c t \gg 1$ the primary contribution will be where both blips and sojourns have lengths which are very large compared to ω_c^{-1}. Consequently, in this regime it seems very plausible that the full expression for $K_n(t)$ may be legitimately approximated by:

1. Replace everywhere the factor $\left[1 + \omega_c^2(\delta t)^2\right]^{-\alpha} \to \omega_c^2(\delta t)^2$ (where here we denoted the time interval between two times as δt).

2. For all X_{jk} apart from $X_{j,j-1}$ set $X_{jk} = 0$

3. Replace $X_{j,j-1} = \frac{\pi}{2}$

Such replacements were made on intuitive grounds in [25], as well as in the more general setting of $\varepsilon \ne 0$ in [15]. However it should be remarked that such approximations are by no means trivial to justify rigorously for "interesting" times of t, namely those (crudely speaking) of order Δ_r^{-1}. Despite this, in Appendix D.1 [3] Leggett et al. proved that in the limit $\frac{\Delta}{\omega_c} \to 0$ and for $\varepsilon = 0$ such simplifications are rigorously legitimate. For brevity we shall not follow their proof, and leave the possibility open to the reader.

The work done in the third subsection of Appendix A results in the equation below for a nearest neighbour contribution

$$P^{(1)}(t) = \sum_m A_m(\alpha)\psi(\Delta_m t) + C \tag{6.4.2}$$

$$\Delta_m = \Delta_{\text{eff}}[e_m(\alpha)]^{\frac{1}{2-2\alpha}} \tag{6.4.3}$$

$$C = 1 - \sum_m A_m \tag{6.4.4}$$

where ψ is the Mittag-Leffler function defined in the Appendix, namely

$$P_r^{(0)}(y) = P_{\text{coh}}(y) + P_{\text{inc}}(y) \equiv \psi(y) \tag{6.4.5}$$

$$P_{\text{coh}} \equiv \frac{1}{1-\alpha} \cos\left\{\left[\cos\left(\frac{\pi}{2}\frac{\alpha}{1-\alpha}\right)\right]y\right\} exp\left\{-\left[\sin\left(\frac{\pi}{2}\frac{\alpha}{1-\alpha}\right)\right]y\right\} \tag{6.4.6}$$

$$P_{\text{inc}} \equiv -\frac{\sin(2\pi\alpha)}{\pi} \int_0^\infty dz \frac{z^{2\alpha-1}e^{-zy}}{z^2 + 2z^{2\alpha}\cos(2\pi\alpha) + z^{4\alpha-2}} \tag{6.4.7}$$

We briefly remark in Appendix A.3 on the Quality factor of the coherent oscillations to be found in equation (A.3.25) is independent of the timescale Δ_{eff} and is defined as

$$Q = 2\pi \times \frac{\text{Energy Stored}}{\text{Energy Dissipated per Cycle}} = \frac{\cos\left(\frac{\pi}{2}\frac{\alpha}{1-\alpha}\right)y}{\sin\left(\frac{\pi}{2}\frac{\alpha}{1-\alpha}\right)y} = \cot\left(\frac{\pi}{2}\frac{\alpha}{1-\alpha}\right) \tag{6.4.8}$$

as such it is clear that in the limit $\alpha \to 0$ the system is completely undamped, in contrast to at $\alpha = \frac{1}{2}$ where the system is overdamped. This value is interesting with regards decoherence since it measures the amount of oscillations, and as such time, it takes for the initial information to be lost as a result of damping caused by the environment. The constant C in (A.3.68) is annoying since it implies $p \not\to 0$ as $t \to \infty$ which we would intuitively expect to hold true. However numerical estimates do indicate that C does vanish up to the accuracy of such calculations [3].

Moreover, we intuitively expect the Markov approximation to be suspect here, so it would be useful if we could generalise our results to account for multiple blip interactions. It is gratifyingly easy to generalize this last work to take into interactions

up to a distance L. By using $r_n^{(l)}(\alpha)$ as an obvious generalization of the quantity $r_n^1(\alpha)$ in A.3, we get a similar equation to there, namely

$$A_m^{(l)}(\alpha) = Q_l^{-1}(\alpha)[e_m^{(l)}]^l(\nu_m^{(l)} \cdot u)^2 \tag{6.4.9}$$

$$Q^{(l)}(t) = \sum_{m=1}^{\infty} A_m^{(l)} \psi(\Delta_m^{(l)} t) + \Delta P^{(l)}(t) \tag{6.4.10}$$

$$\Delta_m^{(l)} = \Delta_{\text{eff}}[e_m^{(l)}(\alpha)]^{\frac{1}{2-2\alpha}} \tag{6.4.11}$$

where we have used $P^{(l)}(t)$ to denote a polynomial which is both finite and given by

$$\Delta P^{(l)}(t) = \sum_{n=0}^{l-1}(-1)^n \left[\hat{K}_n - \hat{K}_n^{(0)} \sum_m (e_m^{(l)})^n a_m^{(l)} \right] (\Delta_{\text{eff}})^{2n(1-\alpha)} \tag{6.4.12}$$

With our equations for $P^{(l)}(t)$ given by equations (A.3.68) minus the constant C, Leggett et al. [3] showed "in the limit $\alpha \to 0$ and $\alpha \to \frac{1}{2}$ these coefficients vanish except at $m = 1$, while A_1 and $e_1(\alpha)$ both tend to unity", thus we recover our expression for $\psi(y)$ from Appendix A.3 in these limits. It is also shown that for intermediate values of α, the important coefficient $A_1(\alpha)$ is always close to unity, while A_2 is never significantly larger than $\simeq 0.06$ beyond this A_m's are much smaller and therefore negligible.

As such we have, in a convoluted way, demonstrated the appropriateness of applying the Non-Interacting Blip approximation in this region. Firstly we ignored the inter-sojourn correlations on purely intuitive grounds. we next showed that in the limits $\alpha \to 0$ and $\alpha \to \frac{1}{2}$ the corrections from including blips were of order α^2 and $(1 - 2\alpha)$ respectively. Finally, we obtain a numerical estimate including nearest-neighbour interactions for α intermediate between 0 and $\frac{1}{2}$ and demonstrate that this is negligible over the first few cycles. It's a natural result that as $\alpha \to 0$ the system is undamped, but now we have a way of obtaining a quantitative value for the rate of damping for multiple blip interactions. This is a very valuable result to those interested in the dynamics of the Spin-Boson model and is possibly the key region of phase-space for those interested in quantum computing.

6.5 Results for the Entire Parameter Space in the Non Interacting Blip Approximation

Previously we have shown that the Non Interacting Blip approximation gives exact results for all T on the line $\alpha = \frac{1}{2}$ and for $\frac{\alpha kT}{\hbar} \gg \Delta_r$ and we determined that it is qualitatively very good (at least for long t) at $T = 0$, for $0 < \alpha < \frac{1}{2}$. Since all areas of phase space are intermediary to these, it is highly plausible that the approximation is valid for all the parameter space. As such, without further justification we apply the Non Interacting Blip approximation in a unified manner. We will along the way obtain some of the results already quoted as special cases to ensure consistency.

As we demonstrated at the end of the last chapter, the quantity $P(t)$ in the Non Interacting Blip approximation is given as the inverse-Laplace transform of $\tilde{P}(\lambda)$, where

$$\tilde{P}(\lambda) = \sum_{n=0}^{\infty}(-1)^n \frac{[f(\lambda)]^n}{\lambda^{n+1}} = [\lambda + f(\lambda)]^{-1} \tag{6.5.1}$$

$$f(\lambda) = \Delta^2 \int_0^{\infty} \cos\left[\frac{q_0^2}{\pi\hbar}Q_1(t)\right] exp\left\{-[\lambda t + \frac{q_0^2}{\pi\hbar}Q_2(t)]\right\} dt \tag{6.5.2}$$

where inserting our equations for $Q_1(t)$ and $Q_2(t)$ in the ohmic case, we find

$$f(\lambda) = \Delta^2 \int_0^{\infty} \frac{\cos\left[2\alpha \tan^{-1}(\omega_c t)\right]}{(1 + \omega_c^2 t^2)^{\alpha}} \left[\frac{\beta\hbar}{\pi t}\sinh\left(\frac{\pi t}{\beta\hbar}\right)\right]^{-2\alpha} exp\{-\lambda t\}$$

$$= \Delta^2 \int_0^{\infty} e^{-\lambda t} \frac{\cos[2\alpha \tan^{-1}(\omega_c t)]}{(1 + \omega_c^2 t^2)^{\alpha}} \left[\frac{\gamma t}{\sinh(\gamma t)}\right]^{2\alpha} dt \tag{6.5.3}$$

where we have defined $\gamma = \frac{\pi}{\beta\hbar}$. We are concerned with the dynamics of $P(t)$ for those times $t \gg \omega_c^{-1}$, as such we need only know $f(\lambda)$ asymptotically where $|\frac{\lambda}{\omega_c}| \ll 1$. To discover this we rewrite the temperature independent factor of (6.5.3) .

Firstly we note

$$\tan^{-1}(x) = \frac{i}{2}\ln\left(\frac{(1-ix)}{(1+ix)}\right) \Rightarrow 2\alpha \tan^{-1}(\omega_c t) = i\ln\left(\frac{(1-i\omega_c t)}{(1+i\omega_c t)}\right)^{\alpha} \tag{6.5.4}$$

and also that $\cos(x) = \text{Re}\left(e^{ix}\right)$, meaning

$$\cos[2\alpha \tan^{-1}(\omega_c t)] = \text{Re}\left(\frac{1+i\omega_c t}{1-i\omega_c t} \cdot \frac{1}{(1+i\omega_c t)(1-i\omega_c t)}\right)^{\alpha} = \text{Re}(1 - i\omega_c t)^{-2\alpha} \tag{6.5.5}$$

from which we update equation (6.5.3) to be of the form

$$\mathrm{Re}\left(\Delta^2 \int_0^\infty (1 - i\omega_c t)^{-2\alpha} e^{-\lambda t}\left[\frac{\gamma t}{\sinh(\gamma t)}\right]^{2\alpha} dt\right) \tag{6.5.6}$$

If we multiply both top and bottom by $(-i\omega_c)^{2\alpha}\lambda^{2\alpha}$ then we obtain

$$\mathrm{Re}\left(\Delta^2 (-i\omega_c)^{-2\alpha}\lambda^{2\alpha} e^{-\lambda t}\left[\frac{\gamma t}{\sinh(\gamma t)}\right]^{2\alpha}\left(\lambda t + \frac{i\lambda}{\omega_c}\right)^{-2\alpha} dt\right) \tag{6.5.7}$$

which when we change variables by setting $t = \lambda^{-1}\left[z - \frac{i\lambda}{\omega_c}\right]$, in turn meaning $dt = \lambda^{-1}dz$, gives us

$$= \mathrm{Re}\left(\Delta^2(-i\omega_c)^{-2\alpha}\lambda^{2\alpha-1}\int_{\frac{i\lambda}{\omega_c}}^\infty z^{-2\alpha} e^{-z} e^{\frac{i\lambda}{\omega_c}}\left[\frac{\left(\frac{\gamma}{\lambda}\right)\left(z - \frac{i\lambda}{\omega_c}\right)}{\sinh\left[\left(\frac{\gamma}{\lambda}\right)\left(z - \frac{i\lambda}{\omega_c}\right)\right]}\right]^{2\alpha} dz\right)$$

$$= \mathrm{Re}\left(\frac{\Delta^2}{(-i\omega_c)^{2\alpha}} e^{\frac{i\lambda}{\omega_c}}\lambda^{2\alpha-1}\int_{\frac{i\lambda}{\omega_c}}^\infty \frac{e^{-z}}{z^{2\alpha}}\left[\frac{\left(\frac{\gamma}{\lambda}\right)\left(z - \frac{i\lambda}{\omega_c}\right)}{\sinh\left[\left(\frac{\gamma}{\lambda}\right)\left(z - \frac{i\lambda}{\omega_c}\right)\right]}\right]^{2\alpha} dz\right) \tag{6.5.8}$$

This can now be expanded using standard methods. We are primarily interested in the leading term, this is obtained by setting $\frac{\lambda}{\omega_c} = 0$ throughout, the resulting integral is tabulated as formula 3.154.1 in [14]. The final result is:

$$f(\lambda) \simeq \frac{\Delta^2}{\omega_c}\left[\left(\frac{2\gamma}{\omega_c}\right)^{2\alpha-1}\cos\left(\alpha\pi + \frac{\lambda}{\omega_c}\right)\frac{\Gamma(1-2\alpha)\Gamma\left(\alpha + \frac{\lambda}{2\gamma}\right)}{\Gamma\left(1 - \alpha + \frac{\lambda}{2\gamma}\right)}\right]$$

$$+ \frac{\Delta^2}{\omega_c}\left[(1-2\alpha)^{-1}\sin\left(\frac{\lambda}{\omega_c}\right) - (2-2\alpha)^{-1}\left(\frac{\gamma}{\omega_c}\right)\cos\left(\frac{\lambda}{2\omega_c}\right) + O\left(\frac{\lambda}{\omega_c}\right)^{2,1+2\alpha}\right] \tag{6.5.9}$$

We remark that this expression is finite in the limits $\alpha \to \frac{1}{2}$, $\alpha \to 1$ and $\gamma \to 0$ etc. To retain the spirit of the Non Interacting Blip approximation we do not want to retain terms of order $\lambda\left(\frac{\Delta}{\omega_c}\right)^2$. Therefore, for α not too close to an integer we impose the following approximations

$$\sin\left(\frac{\lambda}{\omega_c}\right) = \frac{\lambda}{\omega_c} + O\left(\frac{\lambda}{\omega_c}\right)^3 \qquad\qquad \cos\left(\frac{\lambda}{\omega_c}\right) = 1 + O\left(\frac{\lambda}{\omega_c}\right)^2$$

$$\cos\left(\alpha\pi + \frac{\lambda}{\omega_c}\right) = \cos(\alpha\pi)\cos\left(\frac{\lambda}{\omega_c}\right) - \sin(\alpha\pi)\sin\left(\frac{\lambda}{\omega_c}\right) \simeq \cos(\alpha\pi) - \frac{\lambda}{\omega_c}\sin(\alpha\pi) \tag{6.5.10}$$

which, when we substitute these back into (6.5.9) and set coefficients of order unity to one leaves us with

$$f(\lambda) = \Delta_{\mathrm{eff}}\left(\frac{2\gamma}{\Delta_{\mathrm{eff}}}\right)^{2\alpha-1}\frac{\Gamma\left(\alpha + \frac{\lambda}{2\gamma}\right)}{\Gamma\left(1 - \alpha + \frac{\lambda}{2\gamma}\right)} + O\left[\lambda\left(\frac{\Delta}{\omega_c}\right)^2\right] \tag{6.5.11}$$

It is now relatively simple to show that equation (6.5.11) along with earlier definitions coincides with our previous results. For $\lim_{t\to 0} f(\lambda)$ and $\alpha = \frac{1}{2}$ then $f(\lambda)$ reduces to simply Δ_{eff}. As such

$$P(t) = \frac{1}{2\pi i}\int_{-\infty}^\infty e^{i\lambda t}[i\lambda + \Delta_{\mathrm{eff}}]^{-1} d\lambda \tag{6.5.12}$$

has its only singularity of the integrand at $i\lambda = -\Delta_{\mathrm{eff}}$ and as such using the Cauchy residue Formula, as well as the fact that for $|\lambda| \gg 1$ the integrand tends to 0, we have

$$P(t) = e^{-\Delta_{\mathrm{eff}}t} \tag{6.5.13}$$

as anticipated. Similarly for high temperatures ($\gamma \gg 1$), $f(\lambda)$ is observed as varying on a scale which is determined by γ, this allows us to Taylor expand the function around $\lambda = 0$ leaving (in Sect V.F [3])

$$f(\lambda) \simeq f(0)\left[1 - \frac{\pi}{2\gamma}\cot(\pi\alpha)\lambda + ...\right] \tag{6.5.14}$$

where

$$f(0) = \Delta_{\text{eff}} \left(\frac{2\gamma}{\Delta_{\text{eff}}} \right)^{2\alpha-1} \frac{\Gamma(\alpha)}{\Gamma(1-\alpha)}$$

$$= \frac{\Delta^2}{\omega_c} \left[\frac{\pi kT}{\hbar \omega_c} \right]^{2\alpha-1} \frac{\Gamma(\alpha)}{\Gamma\left(\frac{1}{2}+\alpha\right)} \frac{\sqrt{\pi}}{2} \qquad (6.5.15)$$

which means we are left with

$$P(t) \simeq \frac{1}{2\pi i} \int_C e^{\lambda t} \left[\lambda + f(0) \left[1 - \frac{\pi}{2\gamma} \cos(\pi\alpha)\lambda \right] \right]^{-1} d\lambda \qquad (6.5.16)$$

Noting that $f(0)$ is identical to τ^{-1} which we defined earlier, we find we have a singularity in the integrand at

$$\lambda = -\frac{f(0)}{\left(1 - f(0)\frac{\pi}{2\gamma}\cot(\pi\alpha) \right)} = -\frac{\tau^{-1}}{\left(1 - \tau^{-1}\frac{\pi}{2\gamma}\cot(\pi\alpha) \right)}$$

$$= \frac{1}{\left(\frac{\pi}{2\gamma}\cot(\pi\alpha) - \tau \right)} \qquad (6.5.17)$$

which in turn allows us to evaluate $P(t)$ to be

$$P(t) \simeq \frac{1}{1 - f(0)\frac{\pi}{2\gamma}\cot(\pi\alpha)} exp\left\{ -t\frac{f(0)}{1 - f(0)\frac{\pi}{2\gamma}\cot(\pi\alpha)} \right\} \qquad (6.5.18)$$

which we finally rewrite into the form

$$P(t) \simeq \left[1 - \frac{\hbar}{2kT\tau}\cot(\pi\alpha) \right]^{-1} exp\left\{ -\frac{t}{\tau - \frac{\hbar\cot(\pi\alpha)}{2kT}} \right\} \qquad (6.5.19)$$

The terms which here involve $\left(\frac{kT\tau}{\hbar}\right)^{-1}$ are seen to be the first order corrections to our earlier results since they arise from the second term in our Taylor expansion, they form a criterion for what is required to constitute "high temperature", i.e. we demand that these terms are negligibly small.

$$\frac{\hbar}{kT\tau} \ll 1 \Rightarrow \left(\frac{\hbar}{kT} \right)^{2\alpha-2} \ll \frac{\omega_c}{\Delta^2} \frac{2}{\sqrt{\pi}} \frac{\pi^{1-2\alpha}}{\omega_c^{1-2\alpha}} \frac{\Gamma\left(\alpha+\frac{1}{2}\right)}{\Gamma(\alpha)} \tan(\pi\alpha) \qquad (6.5.20)$$

We set terms of order unity to one and rearrange into the form

$$\left(\frac{kT}{\hbar} \right) \gg \left(\frac{\Delta^2}{\omega_c^{-2\alpha}} \right)^{\frac{1}{2-2\alpha}} \left(\frac{\Gamma(\alpha)\pi}{\Gamma\left(\alpha+\frac{1}{2}\right)\tan(\pi\alpha)} \right)^{\frac{1}{2-2\alpha}}$$

$$\Rightarrow \left(\frac{kT}{\hbar} \right) \gg \Delta_r \left(\frac{\pi\Gamma(\alpha)}{\Gamma\left(\alpha+\frac{1}{2}\right)\tan(\pi\alpha)} \right)^{\frac{1}{2-2\alpha}} \qquad (6.5.21)$$

For zero temperature, we must interpret equation (6.5.11) by using Stirling's formula for the gamma function of large arguments, namely

$$\Gamma(z) = \sqrt{\frac{2\pi}{z}} \left(\frac{z}{e} \right)^z \left(1 + O\left(\frac{1}{z} \right) \right) \qquad (6.5.22)$$

which allows us to write

$$f(\lambda) \simeq \lim_{T \to 0} \sqrt{\frac{1-\alpha+\frac{\lambda}{2\gamma}}{\alpha+\frac{\lambda}{2\gamma}}} e^{1-2\alpha} \left(\frac{\lambda}{2\gamma} \right)^{2\alpha-1} \Delta_{\text{eff}} \left(\frac{2\gamma}{\Delta_{\text{eff}}} \right)^{2\alpha-1} \qquad (6.5.23)$$

which leaves us

$$f(\lambda) \simeq \Delta_{\text{eff}}(2\gamma)^{2\alpha-1} \left(\frac{\lambda}{2\gamma} \right)^{2\alpha-1} + O\left[\lambda\left(\frac{\Delta}{\omega_c} \right)^2 \right]$$

$$\simeq \Delta_{\text{eff}}^{2-2\alpha} \lambda^{2\alpha-1} + O\left[\lambda\left(\frac{\Delta}{\omega_c} \right)^2 \right] \qquad (6.5.24)$$

Applying this we find $\tilde{P}(\lambda)$ to be, as we found earlier, the Laplace transform of the Mittag-Leffler function (p.206 [12]). Which recovers our earlier exact results and shows that the application is consistent here as claimed.

6.6   Summary

Where in the earlier chapters we have concluded the chapters with a review of the salient points of the chapter, this is not so important here since this chapter has been one of calculations. Therefore instead what we will do is summarise exactly what we may take away from the results of this chapter. The most obvious conclusion is that the Non-Interacting Blip Approximation is valid for at least some of the phase space in the case of ohmic dissipation, indeed it is exact on the line $\alpha = \frac{1}{2}$, high temperatures or strong dissipation. We have obtained equations which characterise the dynamics under the Non-Interacting Blip approximation although even with this approximation, analysis of the equations is far from trivial. Appendix A more closely considered the dyanmics in particular regions of phase-space.

Appendix A.3 and Sect 6.4 in particular explored the dynamics for the region of phase-space $T = 0$, $0 \leq \alpha < \frac{1}{2}$. This analysis concluded that this region is the most likely to display oscillations between our two states and we obtained from this the quality factor which would be important to us in conceivably obtaining decoherence timescales or other values of interest. Indeed in the region $\alpha \leq \frac{1}{2}$ we obtained several "exact" results, notably under our limits (i.e. $\omega_c \to \infty$), the quantity $P(t)$ depends only on α and the renormalized tunneling frequency Δ_r. We carried out an approximation by considering 'nearest-neighbour' interactions only, and believe that for most practical purposes such an approximation to the correct value is sufficiently accurate over "short times" which we defined with respect to τ in Appendix.A. It is believed that the results which we have replicated in this report are derived from a sufficiently firm basis that with $\alpha \leq \frac{1}{2}$ the case of ohmic dissipation could subsequently be used as a 'test-bed' for theories (analytical or numerical).

We also demonstratred that our work can account for strong dissipation unlike our earlier results using the Born and Markov approxiamtions, although in most practical applications this is unlikely to be useful to us since we would always try and minimise dissipation in our applications. Ultimately we would want to do much more sophisticated analysis of these equations which could help us to accurately model the behaviour of qubits in quantum computing or other applications. In particular we would want to find out the rate of decoherence and dissipation comparing the results to those obtained in the Born-Markov master-equation to see whether for our regions of interest it would not be simpler but nearly as accurate to simply consider those equations. Although this would not be as complex as much of this latest chapter, we refain from doing such an analysis for reasons of space restrictions and expect that the reader would find it reasonably simple to do themselves, or find done in the literature. We now move from this to considering possible applications of decoherence in technology and in particular illuminate the role both decoherence and the Spin-Boson model take in Quantum Computing.

Much of the literature on this problem other than the paper we have followed closely [3] does not concern itself with the quantity $P(t)$ and as such comparison must be approached carefully. Where we briefly discussed possible methods by which one might obtain analogous expressions for the correlation function $C(t)$ many papers calculate this or some other linear-response quantity, even working out equations for $< \hat{\sigma}_z(t) >$ without explicit initial conditions. As such it is unlikely that in these case identical equations would be obtained, however it would be extremely curious and certainly worth further investigation if qualitative features differed, such as oscillations compared to incoherent relaxation.

It is lastly worth mentioning that the particular problem we have concentrated on is quite probably the simplest quantum-mechanical example which displays extreme sensitivity to dissipation whilst simultaneously being in the extreme non-classical limit. It is as such a "crucial test-bed for quantum-mechanical many-body theory and would be important as a model problem even if it had no experimental realizations" (pg.65 [3])

7 Relevance and Applications of Entanglement and Decoherence

In this chapter we will further motivate the interest we attatched to the phenomena of decoherence and entanglement. We shall firstly consider quantum computing by introducing the idea of a "qubit" and proving the no-cloning theorem. This will lead us onto a discussion of combating "noise" in quantum computers where we will consider both Quantum Error-Correcting Codes and Decoherence-Free Subspaces. Finally we will demonstrate a method by which, at least theoretically, entanglement may be used in the field of cryptography. We will closely follow Chapter 7. of [26] which goes into many of the concepts in greater depth than we here have room for.

7.1 Quantum Computers

7.1.1 Qubits and the No-Cloning Theorem

In 'classical' computers, information is encoded in 'bits', where each bit takes either the value 0 or 1. A bit is the unit of information with which a classical computer functions and importantly it is subject to the famous mantra of information theory that "information is inevitably physical" (a phrase which was first emphasized by Landaver). If we consider a quantum system which can take two values such as a spin-$\frac{1}{2}$ particle, to which we attribute the values '0' and '1' then we immediately see the manner in which (ignoring issues such as manipulation of information) we may recover classical computing. However, as discussed in Ch.1, in the quantum realm we are able to achieve superpositions of such states. Herein lies the secret to the popularity of the quantum computer and the quantum bit (qubit) as concepts.

We know that for a qubit with possible base states $|0\rangle$ and $|1\rangle$, we may take any coherent superposition between these states, which when normalised can be expressed as

$$|\psi\rangle = e^{i\phi_0} \cos\left(\frac{\theta}{2}\right)|0\rangle + e^{i\phi_1}\sin\left(\frac{\theta}{2}\right)|1\rangle \tag{7.1.1}$$

where $\theta \, \epsilon \left(0, \frac{\pi}{2}\right)$. In an imprecise way this means that the qubit $|\psi\rangle$ can simultaneously encode both 0 and 1. However, whenever we try and retrieve the information through a measurement, we project the state $|\psi\rangle$ onto the $\{0,1\}$ basis and we are again reduced to the classical case. Thus we must be ingenious in utilising the laws of quantum physics to increasing our computational ability. Let us remove first the overall phase from $|\psi\rangle$ in equation (7.1.1) and thus obtain

$$|\psi\rangle = \cos\left(\frac{\theta}{2}\right)|0\rangle + e^{i\phi}\sin\left(\frac{\theta}{2}\right)|1\rangle \tag{7.1.2}$$

where $\phi = \phi_1 - \phi_0$. In this form it is clear that a qubit is able to encode two values (in our example, θ and ϕ).

Clearly if we made many copies of $|\psi\rangle$, then we could take multiple measurements in many bases and obtain a probability distribution for θ and ϕ. Not only should the idea of a probability distribution rather than a definitive answer worry us, it turns out that no such "cloning" process exists. To demonstrate this we suppose that a device exists, such that

$$|0\rangle_1|\psi\rangle_2 \rightarrow |0\rangle_1|0\rangle_2$$
$$|1\rangle_1|\psi\rangle_2 \rightarrow |1\rangle_1|1\rangle_2 \tag{7.1.3}$$

which is a von-Neumann style evolution equation. Then, since the evolution of the device combined with the qubits is necessarily unitary (due to the unitary nature of the Schrodinger equation), it follows that we have linearity. Meaning

$$\left(|0\rangle_1 + |1\rangle_2\right)|\psi\rangle_2 \rightarrow |0\rangle_1|0\rangle_2 + |1\rangle_1|1\rangle_2 \tag{7.1.4}$$

which is clearly not equivalent to the state

$$\left(|0\rangle_1 + |1\rangle_1\right)\left(|0\rangle_2 + |1\rangle_2\right) = |0\rangle_1|0\rangle_2 + |0\rangle_1|1\rangle_2 + |1\rangle_1|0\rangle_2 + |1\rangle_1|1\rangle_2 \tag{7.1.5}$$

Thereby demonstrating that no process can clone arbitrary quantum bits.

As such, we are still left with the issue of how to access our information without destroying it through a measurement, however we will postpone this discussion and, assuming we can access such information, discuss the advantages of quantum computers. Let us consider a system composed of N qubits meaning we have a Hilbert space of dimension 2^N given by $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes ... \otimes \mathcal{H}_N$, where $\mathcal{H}_i$ is the Hilbert Space of the single qubit $i \, \epsilon \, \{1, ..., N\}$. This means we have 2^N mutually orthogonal basis states which we choose to be of the form

$$|000...0\rangle \equiv |0\rangle_1|0\rangle_2...|0\rangle_N$$
$$|000...1\rangle \equiv |0\rangle_1|0\rangle_2...|1\rangle_N$$
$$... \equiv ...$$
$$|111...1\rangle \equiv |1\rangle_1|1\rangle_2...|1\rangle_N \tag{7.1.6}$$

which we refer to as the computational basis of the N-qubit system. Alternatively if we express the N-qubit state as a density matrix which will be a $2^N \times 2^N$-matrix, we diagonalise this to encode 2^N independent real numbers. This is to be compared

with a classical string of N bits which can only encode N values. As such the first and primary advantage to quantum computers is the exponentially larger storage capacity.

Another advantage comes from consideration of how we may manipulate our qubits. In classical computers, one uses logical gates (such as AND, NOT or XOR) which act on one or two bits at once. By contrast, in the quantum case, we use unitary transformations $\hat{U}$, which act on the Hilbert space of our N-qubit system. This is an important distinction since if we consider an entangled state, then a unitary transformation will effect more than just the single qubit on which it acts, and will probably effect the global state for all N qubits.

For example, let us consider an entangled two-qubit state

$$|\psi\rangle = |0\rangle|1\rangle + |1\rangle|0\rangle \tag{7.1.7}$$

which we subject to the unitary transformation

$$\hat{U} = (|0\rangle\langle 1| - |1\rangle\langle 0|)_1 \otimes \hat{I}_2 \tag{7.1.8}$$

which clearly only alters states in the first Hilbert space. From this we find the transformed state to be

$$\hat{U}|\psi\rangle = -|1\rangle|1\rangle + |0\rangle|0\rangle \tag{7.1.9}$$

If we once again compare this with the classical case, then we find in the classical situation we would have to repeat the operation 2^N times or alternatively run 2^n "processors" in parallel. It can in fact be shown that only one or two quantum gates are required to perform any quantum computation. A particularly useful result since engineering interactions between more qubits than this is difficult.

We finally return to the issue of 'reading out' from a quantum computer. We perform a projective measurement in some chosen basis of some (or all) of our qubits. This will collapse the global state onto some basis vector and destroy all entanglement between the constituent qubits. This firstly means that the possible outcomes must be $\leq 2^N$ and we remain with the probabilistic nature of such a measurement meaning there is a non-zero probability that we will get the wrong answer. This is since even if we have N-qubits which have been identically prepared, the results will vary and as such this may necessitate repeat calculations which have to be considered as intrinsic to the process. Although superficially this seems to invalidate quantum computers since in general we would not necessarily obtain the correct answer, it is usually very simple to verify whether we do have the correct output. As such, provided the probability of obtaining the correct state in the final measurment is sufficiently high meaning we do not require a number of trials which grows exponentially with the complexity of the problem, then we will still have benefitted from the use of quantum computers.

7.1.2 Decoherence in Quantum Computers

As mentioned before in many places, quantum computers derive their power from the existence of superpositions between our basis states. As such, decoherence can reasonably be considered the primary issue to contend with in trying to implement quantum computers. Iit would seem from this discussion to be sufficient to simply shield our qubits from any environmental interactions. While this certainly does prevent the decoherence of the qubits it raises the issue of how we intend to control and manipulate the qubits? A quantum computer that shields the qubits from decoherence but is unable to function is of as little use as one which we are able to control through interaction with some external apparatus, but for which our superpositions rapidly decohere. As such the problem facing those who wish to create a quantum computer comes from satisfying these two opposing demands.

The creation of entanglement between system and apparatus seems an unavoidable consequence of applying unitary operations to our qubits. As such we will investigate the ways in which scientists combat this induced decoherence, such as quantum error-correctiong codes (QEC-codes) and decoherence-free subspaces (DFSs). It is hoped that tools such as these will prevent decoherence from rendering our computer classical, whilst at the same time allowing manipulation of the qubits allowing the quantum computers to maintain their superiority over their classical counterparts.

We note here, that while much of the theory of QEC-codes and DFSs is quite advanced, the implementation of such theories is still in its infancy. While progress is being made such as the experimental implementation of a QEC-code called the "three-bit code" described in [20], the realization of a quantum computer which can rival let alone surpass current classical computers, is still a long way off.

The above introduction to quantum computing has been deliberately both vague and abstract. We have assumed that we can manipulate a set of qubits through the application of unitary transformations (gates). We have avoided being drawn into the details for such gates or even the nature of the qubits, be they polarized photons or spin-$\frac{1}{2}$ particles. The field of creating prototype quantum computers, by which we mean systems of relatively few qubits which can be controlled, is growing rapidly and any attempt to capture this subject would be well outside the scope of this paper. Given this we will continue assuming that such actions are feasible without giving details, and continue to investigate those aspects of quantum computing most pertinent to our subject, quantum error-correction codes and decoherence-free subspaces.

7.1.3 Quantum Error Correcting Codes

There are logically two ways to combat the effects of decoherence on our system. We could try to minimize the effect of decoherence and thereby prevent it from corrupting our coherent superposition state of the qubits. This could be achieved

by encoding in a subspace of the Hilbert space which is immune (or at least approximatley immune) to decoherence, and we will discuss this possibility later. The second complimentary method for combating decoherence involves actively trying to "undo" the errors, analogously to classical error-correction. A genuine time-reversal process would require full control of the environment and is thus completely impractical. However, through the use of an auxilliary system which we couple the system-environment composite to, we can reconstruct the original superposition. Below we will show an example of this scheme which has come to be known under the heading of quantum error-correction. The primary difference between this and classical error-correction is that in the classical case we may simply observer the information which we cannot do in the quantum case since by an observation we would decohere the state and instantly lose the very information we were trying to protect. Meaning we have to correct the induced errors without 'looking' at the information.

Let us firstly emphasize that QEC-codes will be an utterly indispensible tool of any implementation of quantum computing. Even the most optimistic current estimates maintain that without it, decoherence induced, for example, through interactions with the control apparatus, environment or faulty gate operations will simply be too strong for any meaningfully complex quantum computations to be achieved without error-correction. this was exemplified in a comparitively basic computational task which was used by Miquel, Perazzo and Paz [5] and Miquel, Zurek and Paz [6]. The authors used a model of an ion-trap quantum computer which constituted 18 ions (the qubit system) which they used to implement Shor's factorization Algorithm [3] [4] [22] through approximately 15'000 gate operations which were represented physically using laser pulses which acted on the ions. Errors were induced through decoherence resulting from interaction with the environment as well as imperfections in the implementation of gate operations. These models demonstrated that even for low numbers (the authors used 15) the calculation would go rapidly awry, meaning that implementing the algorithm in practce would be impossible.

Taking this as sufficient motivation for our interest in QEC-codes, we note immediately that we cannot carry over the methods of classical error correction. Not only can we not redundantly encode the information as a result of the no-cloning theorem, even if we could this would not directly assist us. As mentioned earlier, we cannot simply observe our N-qubit system, since this would necessarily collapse it to one of the basis-states and we would have lost the very information that we were endeavouring to preserve. As a result of this, it seems apparent that in order to do quantum-error detection, we must not extract information regarding the state itself while we resolve the nature of the error. Therefore, had we redundantly encoded the information contained in our qubit, we would still have no way in which to examine and contrast the information between these qubits without decohering them. We will now follow one of the schemes used to overcome such obstacles and thus indicate how we might implement quantum error-correcting codes.

In the classical setting we are limited to discrete bit flips, which contrasts with the quantum setting, where our two real numbers may change continuously. Superficially it would therefore appear that we would need an uncountably infinite number of separate error-correcting operations. As such, the first hurdle we must overcome is to discretise the continuum of possible errors and thereby reduce it to a manageable number. The fact that this is possible lies at the heart of quantum error correction.

Let us begin by considering a single qubit S which interacts with an environment ε. We express our qubit in a pure-state superposition

$$|\psi\rangle = A|0\rangle + B|1\rangle \tag{7.1.10}$$

subsequently we write the system-environment composite stae as $|\psi\rangle|E_r\rangle$ in the form introduced in Chapter 2. Allowing an interaction to occur between the system and environment which we express arbitrarily as

$$|0\rangle|e_r\rangle \to C_{00}|0\rangle|e_{00}\rangle + C_{01}|1\rangle|e_{01}\rangle$$
$$|1\rangle|e_r\rangle \to C_{10}|0\rangle|e_{10}\rangle + C_{11}|1\rangle|e_{11}\rangle \tag{7.1.11}$$

where $C_{ij} \epsilon \{0, 1\}$ and we have not made requirements such as orthonormality on our states $|e_{ij}\rangle$. Clearly the case of $C_{ij} = \delta_{ij}$ would correspond to a von-Neumann style measurement and thus entanglement (see Ch.2)

We shall consider 'the most general case', namely the one where we take all coefficients equal to one. As such

$$|\psi\rangle|e_r\rangle \to A\left[|0\rangle|e_{00}\rangle + |1\rangle|e_{01}\rangle\right] + B\left[|0\rangle|e_{10}\rangle + |1\rangle|e_{11}\rangle\right] \tag{7.1.12}$$

which we trivially rewrite as

$$|\psi\rangle|e_r\rangle \to (A|0\rangle + B|1\rangle)\frac{1}{2}\left[|e_{00}\rangle + |e_{11}\rangle\right] + (A|1\rangle + B|0\rangle)\frac{1}{2}\left[|e_{01}\rangle + |e_{10}\rangle\right]$$
$$+ (A|0\rangle - B|1\rangle)\frac{1}{2}\left[|e_{00}\rangle - e_{11}\rangle\right] + (A|1\rangle - B|0\rangle)\frac{1}{2}\left[|e_{01}\rangle - |e_{10}\rangle\right] \tag{7.1.13}$$

Where we now observe that each of the terms relating to S may be writtwn as either the identity operator or alternatively one of the Pauli Spin operators acting on $|\psi\rangle$. Which gives us

$$|\psi\rangle|e_r\rangle \to \left(\hat{I}|\psi\rangle\right)\frac{1}{2}\left[|e_{00}\rangle + |e_{11}\rangle\right] + (\hat{\sigma}_x|\psi\rangle)\frac{1}{2}\left[|e_{01}\rangle + |e_{10}\rangle\right] + (\hat{\sigma}_z|\psi\rangle)\frac{1}{2}\left[|e_{00}\rangle - |e_{11}\rangle\right] + (\hat{\sigma}_y|\psi\rangle)\frac{1}{2}\left[|e_{01}\rangle - |e_{10}\rangle\right] \tag{7.1.14}$$

This means that we are able to summarize the result in a satisfactorily compact manner. An arbitrary evolution may as such be expressed as,

$$|\psi\rangle|e_r\rangle \to \hat{I}|\psi\rangle|e_I\rangle + \sum_{s=x,y,z} (\hat{\sigma}_s|\psi\rangle)|e_s\rangle \tag{7.1.15}$$

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[3]Shor's algorithm runs on a quantum computer and, informally, is designed to solve the problem "For a given number N, find its prime factors".

where e_I and $\{|e_s\rangle\}$ are clearly the environmental states which we introduced above, which we recall are not necessarily normalized or orthogonal.

Essentially what this tells us is that an arbitrary influence acting on the qubit from the environment can be written as a weighted sum in the Pauli spin-operators and the identity operator. Such a discretisation is possible since our four operators $\left\{\hat{I}, \hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z\right\}$ form a complete set on the Hilbert Space of our system. It will become apparent how important such a result is in the following work.

If we consider the effect of $\hat{\sigma}_x$ and $\hat{\sigma}_z$ on our qubit it becomes apparent why they are commonly referred to as a "bit-flip" and a "phase-flip"-error respectively

$$\hat{\sigma}_x \left(A|0\rangle + B|1\rangle\right) = A|1\rangle + B|0\rangle$$
$$\hat{\sigma}_z \left(A|0\rangle + B|1\rangle\right) = A|0\rangle - B|1\rangle \tag{7.1.16}$$

i.e. $\hat{\sigma}_x$ swaps the two bits $|0\rangle$ and $|1\rangle$, whereas $\hat{\sigma}_z$ has the effect of rotating the bit $|1\rangle$ by $e^{i\pi}$ which amounts to a sign-flip. The standard relations between the Pauli spin-operators mean that we can express the operator $\hat{\sigma}_y$ as a combination of a "phase-flip" and a "bit-flip" i.e.

$$-i\hat{\sigma}_y = \hat{\sigma}_x \hat{\sigma}_z \tag{7.1.17}$$

However, despite this seeming ability to reduce our consideration to only two Pauli operators we exercise caution and note that such an interpretation is valid iff the relative states of the environment are orthogonal. Only in this case do the Pauli operators represent error probabilities which are mutually exclusive.

In this report we will limit ourselves to consideration of a simplified problem where we only consider environmental entanglement, and therefore by our above reasoning it is clear we need only consider evolution using $\hat{I}$ and $\hat{\sigma}_z$. Meaning

$$|\psi\rangle|e_r\rangle \rightarrow \frac{1}{\sqrt{2}} \left(\hat{I}|\psi\rangle|e_+\rangle + \hat{\sigma}_z|\psi\rangle|e_-\rangle\right) \tag{7.1.18}$$

with

$$|e_\pm\rangle \equiv \frac{1}{\sqrt{2}} \left(|e_{00}\rangle \pm |e_{11}\rangle\right) \tag{7.1.19}$$

We may ind this unsuprising, since decoherence, as explained in Ch.2, is manifest in the delocalization of the local phase relations, meaning that we would intuitively expect "phase-flip errors" to be important.

It is clear that if we denote the operators $\hat{E}_i$ to represent opeators acting on a N-qubit state, for example as

$$\hat{E}_i = \hat{I}^{(1)} \otimes \hat{\sigma}_z^{(2)} \otimes \hat{\sigma}_x^{(3)} \otimes ... \otimes \hat{I}^{(N)} \tag{7.1.20}$$

where we have used the superscript to indicate on which qubit the constituent operators act. Analogously to the single qubit case, when considering entanglement with the environment, we can reduce our considerations to merely operators comprising $\hat{I}$ and $\hat{\sigma}_z$.

In an effort to make our notation both more compact and more transparent we express our operators $\hat{E}_i$ as $\hat{Z}_{j_1, j_2, ..., j_N}$, where $j_k = 0$ if we have $\hat{I}^{(k)}$ or $j_k = 1$ for $\hat{\sigma}_z^{(k)}$.

From this it is clear that a purely entangling system-environment interaction can be written as

$$|\psi\rangle|e_r\rangle \rightarrow \left\{\sum_{j_1=0}^{1} \sum_{j_2=0}^{1} ... \sum_{j_N=0}^{1} \hat{Z}_{j_1, j_2, ..., j_N}|\psi\rangle\right\} |\tilde{e}_{j_1, j_2, ..., j_N}\rangle \tag{7.1.21}$$

where $|\tilde{e}_{j_1, j_2, ..., j_N}\rangle$ are the states of the environment which relate to $\hat{Z}_{j_1, j_2, ..., j_N}$. In the "worst-case scenario" of the environmental entanglement, 2^N distinct $\hat{Z}_{j_1, j_2, ..., j_N}$ would have to be considered, however we shall consider phase-flips upto some weight k, where we define the weight to be the number of single-qubit operators within $\hat{Z}_{j_1, j_2, ... j_N}$ which differ from the identity operator.

Two cases of interest are covered by this assumption, firstly partial decoherence where a small number $k < n$ qubits become entangled allowing us to restrict our attention to 2^k possible error operations of weight $\leq k$. the other case of interest being that of independent qubit decoherence, where we consider a collection of independent phase-flip errors acting on single qubits. Such an approximation is legitimate in situations where a qubit becomes entangled predominantly with its own envionment and the environments do not interact, for example if the qubits are spatially distinct.

Given this let us demonstrate an example of a quantum error-correcting code. Instead of attempting to discover what error was made through measurement of the system and subsequent manipulation of the system-environment, we will employ an extra set of qubits, called an "ancilla", which assists us in detection and correction. These ancilla qubits effectively act as an artificial environment upon which we perform manipulations, and on which we assume we have perfect control.

We once again express the influence of the environment on our system as

$$|\psi\rangle|e_r\rangle \rightarrow \sum_i \left(\hat{E}_i|\psi\rangle\right) |e_i\rangle \tag{7.1.22}$$

where we now attempt to recapture $|\psi\rangle$, To achieve this we use the ancilla qubits $\{|a_i\rangle\}$ as a diagnostic tool. We allow the evolution

$$|a_r\rangle \left[\sum_i \left(\hat{E}_i|\psi\rangle \right) |e_i\rangle \right] \rightarrow \sum_i |a_i\rangle \left(\hat{E}_i|\psi\rangle \right) |e_i\rangle \tag{7.1.23}$$

Which is a von-Neumann style interaction, importantly having no effect on the system, an assumption one may well question. We assume that the $\langle a_i|a_j\rangle \approx 0$, such that the ancilla states can be approximately distinguished upon measurement. We now continue by measuring

$$\hat{O}_A = \sum_i a_i |a_i\rangle\langle a_i| \tag{7.1.24}$$

which acts on the ancilla system, yielding a result a_k. This reduces the whole ancilla-system-environment composite to the state

$$|a_k\rangle \left(\hat{E}_k|\psi\rangle \right) |e_k\rangle \tag{7.1.25}$$

This means that since we know the result was a_k, we know that we must use $\hat{E}_k^{-1}$ to undo the decoherence error, application of which yields

$$|a_k\rangle \left(\hat{E}_k|\psi\rangle \right) |e_k\rangle \longrightarrow \hat{E}_k^{-1} \longrightarrow |a_k\rangle|\psi\rangle|e_k\rangle \tag{7.1.26}$$

Therefore reaching the intended end product, namely our system is rturned to the state $|\psi\rangle$.

It is important to note that throughout this process we have obtained no information about the state of the system, we merely used the ancilla as a sink for the entropy before restoring our original state. We finally remark that this is a highly idealized example with three main issues

- It is not possible that we may design an ancilla system able to distinguish all possible errors.

- the $\hat{E}_i$ are like to be extremely complex, and the jury are still out as to whether the counter-transformations which necessarily require interaction with macroscopic devices, may be implemented without causing excessive decoherence itself.

- The ancilla qubits are subject to the same problems as the computational qubits and decoherence of the ancilla qubits would invalidate our model.

We will not discuss these issues here since they are (predictably) large issues. The interested reader will find a wealth of material available, in particular in Ch 7. of [26] having discussed the above example in slightly more depth Schlosshauer goes on to discuss "When does an Error-Correcting Code exist?". We on the other hand, now turn to our second combating method, namely decoherence-free subspaces.

7.1.4 Decoherence-Free Subspaces

The fundamental idea behind decoherence-free subspaces (DFSs) are that such subspaces $\mathcal{H}_{DF} \subseteq \mathcal{H}$ such that the state $|\psi\rangle \,\epsilon\, \mathcal{H}_{DF}$ remain (exactly or approximately) coherent and pure, despite environmental interactions. DFSs effectively allow us to encode our quantum information in what could be termed "quiet corners" of the Hilbert Space. In contrast with error-corrections which we saw above aimed to correct errors, DFSs aim to prevent errors occuring in the first place, thus DFSs represent a stategy for "intrinsic error avoidance".

If we decompose the interaction Hamiltonian for our general system-environment composite into the diagonal representation

$$\hat{H}_{\text{int}} = \sum_\alpha \hat{S}_\alpha \otimes \hat{E}_\alpha \tag{7.1.27}$$

In which case a necessary requirement for the existence of a DFS is a set of orthogonal degenerate eigenstates $|s_i\rangle$. If this is the case then any of our coded states may be expressed as a superposition in our states $|s_i\rangle$

$$|\psi\rangle = \sum_i c_i |s_i\rangle \tag{7.1.28}$$

and these states will evolve as

$$e^{-i\hat{H}_{\text{int}}t}|\psi\rangle|E_0\rangle = e^{-i\hat{H}_{\text{int}}t} \left(\sum_i c_i|s_i\rangle \right) |E_0\rangle$$

$$= \left(\sum_i c_i|s_i\rangle \right) e^{-i\sum_\alpha \lambda^\alpha \hat{E}_\alpha t}|E_0\rangle \equiv |\psi\rangle|E_\psi(t)\rangle \tag{7.1.29}$$

where importantly the state does not become entangled with the environment. It is clear that the self-Hamiltonian $\hat{H}_S$ must be such that a state in a DFS remains so for all time. That is where $|\psi\rangle\epsilon\{|s_i\rangle\}$, then $\hat{H}_S|\psi\rangle\epsilon\{|s_i\rangle\}$, $\forall t \geq 0$. If this were not

the case, then a state initially immune to decoherence would eventually still decohere but on a timescale set by the evolution. These conditions amount to the presence of dynamical symmetries.

We will below consider a very simple example, where all qubits interact identically to the environment and as such the system-environment interaction is symmetric wih respect to any permutation of qubits. However we would ideally like the DFS to be quite robust to small perturbations which come from small additional couplings. Initial work by Lidar, Chuang and Whaley [9] and Bacon, Lidar and Whaley [10] demonstrated that in the order of perturbation strength, while storage in a DFS is stable to all orders in time, processing on the other hand is stable only to first order in time. It was however demonstrated in [8] that combination of these methods with quantum error-correcting codes can mitigate the problem.

Let us initially distinguish the two extremes for modeling decoherence with respect to systems of qubits. Firstly, 'independent decoherence' by which we mean that each and every qubit is linked to its own environment and these environments do not interact. We previously made such an assumption for quantum error correcting codes and indeed this assumption is usually made in the context of quantum error correction. The importance of such an assumption is that if we denote 'p' to be the probability of an error to occur on one qubit, the probability it will happen to k qubits is simply p^k. This allows us to express our qubit errors as a set of single-qubit errors each of weight one, which we then express as a linear combination. This assumption underpins many error-correcting schemes which are only capable of correcting such single-qubit errors.

Let us however consider the situation where our qubits are 'spatially close', then the above assumption is no longer applicable. Where the criteria by which we define 'spatially close' is dependent on the typical decoherence length of the environment. In this case, all qubits experience (more or less) a single environment, meaning we should expect 'bursts' of errors, since errors may well become correlated within multiple qubits. Such a situation is typically termed 'collective decoherence' where all qubits interact with the same environment.

Ultimately, the size of our possible decoherence-free subspace is controlled by these two extremes, independent versus collective decoherence. If we take the spin-boson model (as our most considered example), it turns out that for collective decoherence (and multiple qubits), the dimension of our DFS will asymptotically approach that of the original collective Hilbert Space. As such, in this limit we are permitted optimal decoherence-free encoding. In the opposing limit, that of independent decoherence, no subspace can be found such that it is both free from decoherence and able to encode logical qubits. Although we do not have the space here to establish these facts rigorously, we may demonstrate the connection between the dimension of a DFS and the model we use for decoherence in a simple example.

We start by considering a model for 'collective decoherence' in the spin-boson model. We generalize the interaction Hamiltonian from before to one which encompasses all N qubits in our collection and we write it as

$$\hat{H}_{\text{int}} = \sum_{i=1}^{n} \hat{\sigma}_z^{(i)} \otimes \sum_j \left(g_{ij} \hat{a}_j^\dagger + g_{ij}^* \hat{a}_j \right) \equiv \sum_{i=1}^{n} \hat{\sigma}_z^{(i)} \otimes \hat{E}_i \tag{7.1.30}$$

where we have reintroduced the creation (annihilation) operators $\hat{a}_j \left(\hat{a}_j^\dagger \right)$ which act on the jth-oscillator in the environment and we have also introduced g_{ij} to represent the strength of coupling between the jth-oscillator and i^{th}-qubit. However, once we impose our restriction that all qubits couple to the same environment, then we deduce that

$$\hat{H}_{\text{int}} = \left(\sum_{i=1}^{n} \hat{\sigma}_z^{(i)} \right) \otimes \hat{E} = \hat{S}_z \otimes \hat{E} \tag{7.1.31}$$

where the exact form of $\hat{E}$ is not important, what is important is that we have an interaction Hamiltonian with one term instead of a sum of terms.

At this point we recollect from earlier that a DFS consists of degenerate eigentates of the system under the operator $\hat{S}_z$ of the interaction Hamiltonian. It is evident that we need only express any N-qubit product state with respect to the basis spanned by eigenvectors of $\hat{S}_z$. There are as such clearly 2N+1 different possible eigenvalues for this process ranging from $m = -N$ (which corresponds to the state $|1, 1, ..., 1\rangle$) to $m = N$ (with basis state $|0, 0, ..., 0\rangle$). We generalize this to say that any basis state with m_0 qubits in state '1' will yield the eigenvalue

$$m = N - 2m_0 \tag{7.1.32}$$

Let us now ask the natural question, namely: "What is the largets set of mutually orthogonal basis states which yield the same eigenvector under the action of $\hat{S}_z$" where we call this group $\mathcal{D}_0$. This is quite clearly going to be the case where $m = 0$ meaning we have equal number of qubits in the "0" and "1" states, (for n=odd it will be $m = \pm 1$, meaning only one more in either '0' or '1' state). We express such a set as

$$\mathcal{D}_0 = \left\{ |i_1, i_2, ..., i_N\rangle : i_j \epsilon \{0, 1\}, \sum_{j=1}^{N} i_j = 0 \right\} \tag{7.1.33}$$

where there are $n_0 = \binom{N}{\frac{N}{2}}$-states which are mutually orthogonal and exist in this set. As such this set $\mathcal{D}_0$ is of dimension n_0 and for large values of N we use Stirling's formula to approximate the binomial coefficients to find

$$\log_2 \binom{N}{\frac{N}{2}} \approx N - \frac{1}{2}\log\left(\frac{N\pi}{2}\right) \sim N \tag{7.1.34}$$

which demonstrates that at least for the limiting case of collective decoherence the dimension of our DFS approximately matches that of our original Hilbert space, meaning also that our encoding efficiency tends to unity.

If we consider this case for $N = 6$ we would have a set of 20 basis vectors in our set $\mathcal{D}_0$ which would be our maximum-size DFS, whereas generally the Hilbert space has dimension $2^6 = 64$. As such, given our model for collective decoherence we may encode upto 4 logical qubits in such a DFS. Five logical qubits would need a $2^5 = 32$-dimension state space which we do not have in this instance. As a result we see that we may use 6 logical qubits to enact quantum computations with no more than 4 logical qubits in a decoherence-free manner.

In contrast, considering the case of independent decoherence, we make the following observation. In general, the environment operators denoted $\hat{E}_i$ which appear in (7.1.30) will be distinct from each other. For a DFS we determine a set of basis states $\{|s_i\rangle\}$ which are mutually orthogonal as well as having the property,

$$\left[\hat{I}^{(1)} \otimes ... \otimes \hat{I}^{(j-1)} \otimes \hat{\sigma}_z^{(j)} \otimes \hat{I}^{(j+1)} \otimes ... \otimes \hat{I}^{(N)} \right] |s_i\rangle = \lambda^{(j)} |s_i\rangle \tag{7.1.35}$$

$\forall i, 1 \leq j \leq N$. Which are the interaction-operators for the system in the case of independent decoherence. However, only two such states satisfy this and not simultaneously, either $|00...0\rangle$ or $|11...1\rangle$. Since at least two states are required to exist simultaneously to allow encoding of even a single logical qubit, it follows that no DFS exists for the case of independent decoherence.

Naturally in realistic circumstances neither of these extremes is realised exactly and we must consider a weighted combination of the two. However, we now have two complementary methods which we may use to combat decoherence, namely decoherence-free subspaces and quantum error-correcting codes. we may use DFSs to prevent collective decoherence effects and quantum error correction to recover from single-qubit errors. By joining these two methods it is possible to create universal fault-tolerance quantum computation even were we to relax the restriction permitting only single-qubit errors.

The results of one effort to realize a simple DFS were given in 2001 by Kielpinski et. al. [11]. In this experiment the two-qubit Bell-states were used when the authors encoded the single logical qubit into a DFS of two trapped Be^+ ions which interacted strongly. What was demonstrated was that superpositions of the encoded basis states were immune to collective decoherence, since the observed decoherence was much slower than 'normal' and could be attributed to effects such as the degredation of the read-out pulse. As such this experiment demonstrated an experimental construction of a DFS of 2-dimensions using four physical qubits. Experiments intending to construct larger DFSs using alternate physical qubits have since been attempted, such as Viola et.al. in 2001, who generated the first 3-qubit DFS using NMR qubits [21].

7.2   Quantum Cryptography

Rather than discuss the field of quantum cryptography, which is large and varied, in general terms, we will here mostly use an example to illustrate the general concepts, however we will briefly outline a few key concepts. Cryptography is concerned with allowing two parties to communicate without a third party being able to intercept and understand the information. These people are by custom and practice referred to as Alice and Bob as well as Eve the 'eavesdropper'. We also remark that the 'no-cloning' therorem which we used earlier is important here, since it prevents Eve from intercepting a transmitted quantum state copying it and then sending the original (or the copy) onwards to Bob, the importance of such a result will be obvious later.

We shall follow the BB84 quantum key exchange protocol (so-called since it was first invented by Bennett and Brassard in 1984). In this method Alice communicates either a zero or one to Bob through the use of four non-orthogonal states. The use of non-orthogonal states prevents either Eve or Bob from perfect discrimination, so how can Alice and Bob communicate with immunity from Eve? We now follow an idealized method which will indicate the general idea and manner of quantum cryptography.

Alice transmits photons to Bob, in one of four polarizations as shown in Fig(.) below

Let us imagine that Alice prepares her states in the $\{|+\rangle, |-\rangle\}$-basis then if Bob chooses to measure in this basis he necessarily obtains the same state Alice prepared. if on the other hand Bob measures in the $\{|0\rangle, |1\rangle\}$-basis then he has equal probabilities of measuring a $|0\rangle$ or $|1\rangle$ irrespective of which state was originally encoded in the $\{|+\rangle, |-\rangle\}$-basis. Similarly if Alice encoded a $|0\rangle$ or $|1\rangle$ then Bob can obtain this state by measuring in the correct basis and the states have equal probability of collapsing to a $|+\rangle$ or a $|-\rangle$ if measured in the $\{|+\rangle, |-\rangle\}$-basis.

If Eve measures the states (which she cannot copy for later reference) on their way to Bob, like Bob she has probability $\frac{1}{2}$ of choosing a basis different from the one Alice used for encoding. Assuming Bob then chooses the basis that Alice originally used the state which emerged after Eve will be in the wrong basis and will have a 50-50 chance of collapsing to a state different to the one sent by Alice. Therefore $\frac{1}{4}$ of the time where Bob and Alice have chosen the same basis Bob will get different states as a result of Eve's intervention. This means that if Alice and Bob compare n results where Bob chose the same basis as Alice, then Eve has a $\left(\frac{3}{4}\right)^n$ chance of being detected, i.e. if they compare 20 states then Eve has a probability of less than $\frac{1}{250}$ of not being caught. Then Alice and Bob having satisfied themselves the 'channel' is clear are able to communicate their message secretly as described next. If they find that they are being eavesdropped on, then they may change 'channel' and start over without any information having been gleaned by Eve. As such, this method does not prevent eavesdropping, it simple makes it possible to detect eavesdroppers without revealing the secret information. We now understand the way in which this method prevents eavesdropping so how does it facillitate communication between Alice and Bob?
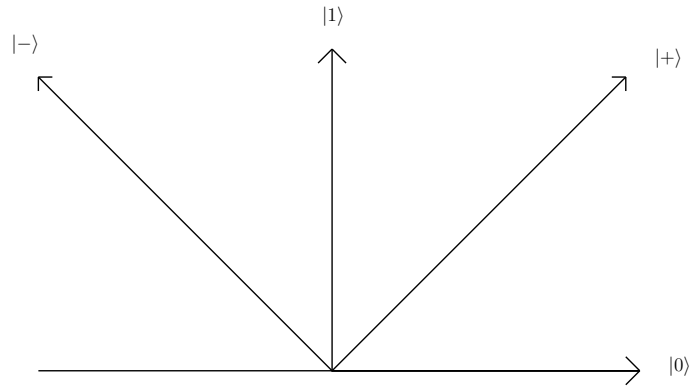
Figure 12: A graphical representation of the computational bases we will use, namely the $\{|0\rangle, |1\rangle\}$ and $\{|-\rangle, |+\rangle\}$-basis.

In the BB84 protocol, Alice chooses a random string $x_1, x_2, ..., x_n$ of bits which she intends to transmit, e.g.

$$
\begin{array}{c|c|c|c|c|c|c}
\text{Bit} & x_1 & x_2 & x_3 & x_4 & x_5 & x_6 \\
\hline
\text{Value} & 0 & 1 & 0 & 0 & 1 & 0
\end{array}
\tag{7.2.1}
$$

Next Alice chooses to encode each bit as a qubit $|\psi_i\rangle$ in one of the two bases $\{|0\rangle, |1\rangle\}$ or $\{|+\rangle, |-\rangle\}$, e.g.

Bit	x_1	x_2	x_3	x_4	x_5	x_6
Basis	0,1	+,-	+,-	0,1	+,-	0,1
Encoding	$|0\rangle$	$|+\rangle$	$|-\rangle$	$|0\rangle$	$|+\rangle$	$|0\rangle$

(7.2.2)

A logical 'one' is encoded as either a $|1\rangle$ or $|+\rangle$ and a logical 'zero' $|1\rangle$ or $|-\rangle$. Alice then transmits this string of qubits to Bob who, choosing his own random string of bases, decodes the string e.g.

Value	x_1	x_2	x_3	x_4	x_5	x_6
Alice's Basis	0,1	+,-	+,-	0,1	+,-	0,1
Bob's Basis	0,1	0,1	+,-	+,-	0,1	0,1
Agreement	Yes	No	Yes	No	No	Yes

(7.2.3)

After this Alice and Bob talk on a public channel and compare the bases they chose for each qubit, NOT the qubit they measured. If an eavesdropper listens to this all they glean is the bases which were used which does not tell Eve the classical value sent/received. Alice and Bob keep only those values for which they used the same basis and as such definitely have the same value for, in our case the string 000 which is unknown to any eavesdropper. This string can now be used as a one-time cipher which is uncrackable without the string or repeats of the string (i.e. using a string of length n to encode a message $> n$). Clearly to check for eavesdroppers requires a reasonable number of qubits and on average, Alice and Bob will randomly select the same basis half the time. Therefore less than half the qubits sent will ultimately be used to encode, meaning lots of excess sending compared to message length. A message of length n with m-qubits checked for eavesdropping will require $2(m+n)$ sent qubits. However, this shows how, at least in principle, quantum mecanics may be utilised to allow secure key exchange between communicating parties.

By March 2007, the largest distance over which quantum mechanics had been used to communicate a key used optical fibres and the BB84 protocol to communicate over 148.7 km by the Los Alamos National Laboratory. However, in free space a European collaboration used the so-called Ekert system with entangled photons to communicate over 144km between two of the Canary islands in 2006. There are also at least 4 companies which offer commercial quantum cryptography, namely id Quantique, MagiQ Technologies, SmartQuantum and Quintessence Labs. From this it should be clear that this area will be a major source of interest in the future.

8 Conclusions

In this report we began by reviewing several phenomena of quantum mechanics from which the important points to emphasise were that there is no classical way to explain either superpositions or entanglement. That is, the observed results in microscopic (and increasingly macroscopic) experiments require a clean break from classical physics, with such results being explained by quantum mechanics. In particular we developed the logic used by Bell to derive an inequality which separates the predictions of 'local hidden variables' from those of the traditional Copenhagen Interpretation of quantum mechanics. Having stressed this break between classical and quantum physics it became natural to ask the question: "How does classical physics emerge as a macroscopic limiting case of the underlying quantum laws?" It was this question that originally motivated our interest in the topic of decoherence, before we began to study it for its own sake.

We next discussed the short-fallings of the traditional operator formalism, from these considerations we described a modified formalism in terms of density matrices and reduced density matrices, alongside a new description of measurement in this formalism which we titled the Ideal von-Neumann Measurement Scheme. It was a short step from this to introducing the concept of decoherence in its most general form. Through this introduction we immediately made two important observations, firstly the nature of the entanglement and therefore the decoherence that occurs is entirely captured in the form of the interaction. This was necessary to avoid any basis ambiguity arising after the event and contradicting the fact that an observer cannot simultaneously measure non-commuting variables. This led us to our second important observation, being that since many (if not most) interactions in nature are a function of position, in the form of separation, then it is this basis which is most commonly 'chosen' in nature. Compare this to an isolated system where the Hamiltonian is diagonal in the energy eigenbasis, which explains why in a closed system this is the basis within which superpositions do not emerge. Put more generally, decoherence explains the mechanism for the emergence of classical physics from the underlying quantum laws.

We next considered a simple model for decoherence called the 'Scattering Model' which we showed, under what might be called 'normal' conditions, decoheres very efficiently. The model was of a macroscopic object scattering microscopic objects (e.g. photons) and we obtained lower bounds on the decoherence rate. The conclusions which we drew from this model that were most important to us were that the decoherence timescale is much shorter than timescales for other physical processes such as dissipation. We also demonstrated that at least for this model, the temperature of the environment and the length of the coherent separation were the most powerful factors, however even an environment at a temperature of 3K would still cause rapid decoherence on a mesoscopic scale.

Having done this we set about describing ways in which we could simplify the process, for more complex examples, of finding the quantities of interest. We concentrated on the tools of master-equations and canonical models. In particular we developed a set of equations which governed the evolution of the so-called Spin-Boson Model under the Born and Markov approximations as described in Ch.4. These equations not only detailed the rate and effect of decoherence on the coherent superpositions, but also the effect of the environment in other physical processes such as dissipation. It would be of interest to compare carefully observed experimental data with the predictions of these equations in different regimes of temperature and coupling strength. Such comparison should validate those assumptions and remarks we made whilst implementing our assumptions, however anomalous regions or results would be particularly interesting since it may indicate the influence of a variable we had not considered.

Due to space restrictions we were unable to delve as deeply into master-equations as would have been ideal. In particular [26] took the work we did into greater depth by considering master-equations other than the Born-Markov example we considered. As well as this Schlosshauer considering the Quantum Brownian Motion model which is fascinating and, since it uses much of the work we did on the environment self-correlation functions, would not require excessive amounts of extra work for the reader, whilst also displaying nicely the different timescales in the position and momentum Wigner representations. We also did not consider spin-environments in the same detail as oscillator-environments and the section on this in the same book is very instructive, considering mapping between oscillator and spin-environments. It also became immediately apparent from this work that the introduction of an interacting environment leads to qualitatively different dynamics to the isolated case.

Our work following this on the Spin-Boson model was technical and sophisticated, ultimately leading to a set of equations which solved the model exactly under certain restrictions which were used to generate the Hamiltonian entirely from physical considerations (see [3]). We justified the Non-Interacting Blip approximation in the ohmic case and thus obtained practically usable equations which were both more accurate and more applicable throughout (α, T)-phase space. It would be very interesting and possibly not too difficult to apply a more sophisticated analysis on the Spin-Boson model. It would seem simplest to analyse the ohmic case since we have already done much of the work, and as remarked in Ch.6 there are many quantities and questions still left to investigate. It almost goes without saying that more careful analysis of almost any of the assumptions we made at any stage of our derivation of these equations would be of interest. It is unlikely that the results would contrast greatly with those we predicted since we were careful to justify our assumptions where possible. However quantitative analysis of the errors induced by each assumption in varying regimes would indicate the assumption which introduced the most error, or most limited our applicability.

Alternatively the subohmic and superohmic cases are still open to the interested reader and a comparison between the cases in different regions of phase space may turn up results which we have not anticipated. We could even try to change the oscillator-environment into a spin-environment analogous to the so-called Kondo model. We noted that at low temperatures spin-environments are more appropriate, this is where the dominant causes of decoherence are nuclear spins or intrinsic

impurities in the environment and object of interest. We remarked at the time, that further exploration of the results of Feynman and Vernon on mapping environments to oscillators provided sufficiently weak interaction, would be very instructive and beneficial when added to the topics here studied. While it requires a sound understanding of the Feynman path integral formalism of quantum mechanics, this is presented clearly in many textbooks and is not difficult for the reader familiar with the Lagrangian formalism of classical physics. Overall it should be clear that this is a near inexhaustible field of possible topics that we have barely touched the surface of.

In the final chapter we briefly considered some of the roles of entanglement and decoherence in quantum technology, such as quantum computers and quantum cryptography. In particular sound understandings of the problems poised by decoherence in quantum computing is essential to an appreciation of the subject. This area is still extremely active and, especially in terms of implementation, in its infancy. Since decoherence is the primary obstacle in implementation of a usable quantum computer, there is a vast array of literature on the topic being published each year, meaning anyone who wished to capture this area would be facing a Herculean task. The reader could however do much worse than consider some of the papers and books mentioned in Ch.7. This will no doubt be a fruitful, ingenious and fascinating region of research in the future with physicists inventing ever more beautiful and elaborate methods of manipulating the laws of quantum mechanics with the hope of building a working quantum computer which can outperform its classical counterpart.

A Justification of Non-Interacting Blip Approximation for the Ohmic Case in the Spin-Boson Model

A.1 General Formulae

We begin by inserting our spectral density $\left(J(\omega) = \eta\omega e^{-\frac{\omega}{\omega_c}}\right)$ into our two equations (5.2.44) and (5.2.45). Thus we start with $Q_1(t)$ and get

$$Q_1(t) = \eta \int_0^{\omega_c} \frac{\sin(\omega t)}{\omega} e^{-\frac{\omega}{\omega_c}} d\omega \tag{A.1.1}$$

let us make the change of variables $\omega t = \tan(\theta)$ which means that $d\omega \to \frac{1}{t}\cos^{-2}(\theta)d\theta$ and gives us

$$Q_1(t) = \eta \int_0^{\tan^{-1}(\omega_c t)} \sin(\tan(\theta))e^{-\frac{\tan(\theta)}{\omega_c t}}(\cos(\theta)\sin(\theta))^{-1}d\theta \tag{A.1.2}$$

Since we know that $\omega_c t$ is not too long in order that we remain in "interesting times", this means $\theta \ll \frac{\pi}{2}$ and as such we express all parts of our integral to lowest order in θ, $\sin(\theta) \sim \theta$, $\tan(\theta) \sim \theta$, $\cos(\theta) \sim 1$ and $e^{-\theta} \sim 1$, which by substitution gives us

$$Q_1(t) \simeq \eta \int_0^{\tan^{-1}(\omega_c t)} \sin(\theta)e^{-\frac{\theta}{\omega_c t}}(\theta\cos(\theta))^{-1}d\theta \simeq \eta \int_0^{\tan^{-1}(\theta\omega_c)} d\theta = \tan^{-1}(\omega_c t) \tag{A.1.3}$$

We next consider the second of our two expressions, namely $Q_2(t)$, inserting $J(\omega)$ gives,

$$Q_2(t) = \int_0^\infty \eta \frac{e^{-\frac{\omega}{\omega_c}}}{\omega}(1 - \cos(\omega t))\coth\left(\frac{\beta\hbar\omega}{2}\right) \tag{A.1.4}$$

We start by rewriting several terms such as $(1 - \cos(\omega t)) \to \omega \int_0^t \sin(\omega t')dt'$ and $\cosh\left(\frac{\beta\hbar\omega}{2}\right) = 1 + 2e^{-\frac{\beta\hbar\omega}{2}}\left(\sinh\left(\frac{\beta\hbar\omega}{2}\right)\right)^{-1}$. As such we change the order of integration and differentiation to get

$$Q_2(t) = \int_0^t dt' \int_0^\infty \eta e^{-\frac{\omega}{\omega_c}}\sin(\omega t')\left(1 + 2e^{-\frac{\beta\hbar\omega}{2}}\left(\sinh\left(\frac{\beta\hbar\omega}{2}\right)\right)^{-1}\right)d\omega \tag{A.1.5}$$

If we consider only the first term here and use integration by parts twice this term becomes

$$\frac{1}{2}\eta \ln(1 + \omega_c^2 t^2) \tag{A.1.6}$$

The second term in equation (A.1.5), namely $\int_0^t dt' \int_0^\infty 2\eta e^{-\frac{\omega}{\omega_c}}\sin(\omega t')\left(2e^{-\frac{\beta\hbar\omega}{2}}\sinh^{-1}\left(\frac{\beta\hbar\omega}{2}\right)\right)d\omega$, when evaluated leaves us with the result

$$Q_2(t) = \frac{1}{2}\eta \ln(1 + \omega_c^2 t^2) + \eta \ln\left[\frac{\beta\hbar}{\pi t}\sinh\left(\frac{\pi t}{\beta\hbar}\right)\right] \tag{A.1.7}$$

where we recall $\beta = \frac{1}{k_\beta T}$ (k_β = Boltzmann constant). It is convenient until further notice to measure time in units of ω_c^{-1}. We can as such evaluate $f(t)$ being the contribution of an isolated blip to the influence functional

$$f(t) = \Delta^2 \cos\left[\frac{q_0^2}{\pi\hbar}Q_1(t)\right]exp\left\{-\frac{q_0^2}{\pi\hbar}Q_2(t)\right\} \tag{A.1.8}$$

and through noting that $\frac{\eta q_0^2}{\pi\hbar} = 2\alpha$, we insert our equations (A.1.3) and (A.1.7) for $Q_1(t)$ and $Q_2(t)$ to obtain,

$$f(t) = \Delta^2 \cos\left[2\alpha\tan^{-1}(t)\right]\left[\left(\frac{\pi t}{\beta\hbar\omega_c}\right)\frac{\text{cosech}\left(\frac{\pi t}{\beta\hbar\omega_c}\right)}{(1 + t^2)^{-\frac{1}{2}}}\right]^{2\alpha} \tag{A.1.9}$$

Note briefly that since $\tan^{-1}(t) < \frac{\pi}{2}$, then $f(t) > 0$ provided that $\alpha \leq \frac{1}{2}$, by contrast if $\alpha > \frac{1}{2}$ then there are oscillations coming from the cosine function.

From this we continue to try and find an expression for $P(t)$ we substitute equations (A.1.3) and (A.1.7) into our equations for $P(t)$ from the previous chapter, and set $\varepsilon = 0$ so that we consider the unbiased case. Firstly we consider F_1, with $S_j = \sum_{j=1}^n b_j$ we find

$$S_j = \sum_j \eta\left[\frac{1}{2}\ln(1 + \omega_c^2 b_j^2) + \ln\left(\frac{\beta\hbar\omega_c}{\pi b_j}\sinh\left(\frac{\pi b_j}{\beta\hbar\omega_c}\right)\right)\right] \tag{A.1.10}$$

which we express as

$$F_1 = \prod_{j=1}^{n} \left[f'(b_j) \right]^{2\alpha} \tag{A.1.11}$$

where we have defined

$$f'(b_j) \equiv (1 + \omega_c^2 b_j^2)^{-\frac{1}{2}} \left(\frac{\beta \hbar \omega_c}{\pi b_j} \sinh \left(\frac{\pi b_j}{\beta \hbar \omega_c} \right) \right)^{-1} \tag{A.1.12}$$

The term F_2 is a function of the variable Λ_{jk} which we can now express as

$$F_2 = \prod_{k=1}^{n-1} \prod_{j=k+1}^{n} \left[\frac{f'(t_{2j} - t_{2k-1}) \cdot f'(t_{2j-1} - t_{2k})}{f'(t_{2j} - t_{2k}) \cdot f'(t_{2j-1} - t_{2k-1})} \right]^{2\alpha \zeta_j \zeta_k} \tag{A.1.13}$$

If we now make the definition,

$$u_{jk} = t_{2j-1} - t_{2k} \tag{A.1.14}$$

then we can write F_2 as a function of u_{jk} and b_j

$$F_2 = \prod_{k=1}^{n-1} \prod_{j=k+1}^{n} \left(\frac{f'(u_{jk} + b_j + b_k) f'(u_{jk})}{f'(u_{jk} + b_j) f'(u_{jk} + b_k)} \right)^{2\alpha \zeta_j \zeta_k} \tag{A.1.15}$$

Combining F_3 and F_4 into one term which we will from now on call F_3 while also recalling that $\varepsilon = 0$ we are left with

$$F_3 = \prod_{k=1}^{n-1} \cos \left[\frac{q_0^2}{\pi \hbar} \sum_{j=k+1}^{n} \zeta_j X_{jk} \right] \cos \left[\frac{q_0^2}{\pi \hbar} \sum_{j=1}^{n} \zeta_j X_{j0} \right] = \prod_{k=0}^{n-1} \cos \left[\frac{q_0^2}{\pi \hbar} \sum_{j=k+1}^{n} \zeta_j X_{jk} \right] \tag{A.1.16}$$

which after substituting our earlier equations for X_{jk} and $Q_1(t)$, leaves us

$$F_3 = \prod_{k=1}^{n-1} \cos \left[2\alpha \sum_{j=k+1}^{n} \zeta_j (\tan^{-1}(t_{2j} - t_{2k+1}) + \tan^{-1}(t_{2j-1} - t_{2k}) - \tan^{-1}(t_{2j} - t_{2k}) - \tan^{-1}(t_{2j-1} - t_{2k+1})) \right] \tag{A.1.17}$$

In an attempt to simplify this last term. We make the definition

$$y_{jk} = t_{2j-1} - t_{2k+1} \tag{A.1.18}$$

which leaves our arctan functions as

$$\tan^{-1}(y_{jk} + b_j) + \tan^{-1}(y_{jk} + s_k) - \tan^{-1}(y_{jk} + b_j + s_k) - \tan^{-1}(y_{jk}) \tag{A.1.19}$$

which by use of the addition formula for arctan, namely $\tan^{-1}(\alpha) \pm \tan^{-1}(\beta) = \tan^{-1}\left(\frac{\alpha \pm \beta}{1 \mp \alpha \beta} \right)$, we express as

$$\begin{aligned} &= \tan^{-1}\left(\frac{-s_k}{1 + (y_{jk} + b_j)(y_{jk} + b_j + s_k)} \right) + \tan^{-1}\left(\frac{s_k}{1 + y_{jk}(y_{jk} + s_k)} \right) \\ &= \tan^{-1}\left(\frac{s_k(1 + (y_{jk} + b_j)(y_{jk} + b_j + s_k)) - s_k(1 + y_{jk}(y_{jk} + s_k))}{s_k^2 + (1 + y_{jk}(y_{jk} + s_k))(1 + (y_{jk} + b_j)(y_{jk} + b_j + s_k))} \right) \\ &= \tan^{-1}\left(\frac{b_j s_k(b_j + s_k + 2y_{jk})}{s_k^2 + (1 + y_{jk}(y_{jk} + s_k))(1 + (y_{jk} + b_j)(y_{jk} + b_j + s_k))} \right) \end{aligned} \tag{A.1.20}$$

substituting into equation (A.1.17) gives,

$$F_3 = \prod_{k=0}^{n-1} \cos \left[2\alpha \sum_{j=k+1}^{n} \tan^{-1}\left(\frac{b_j s_k(b_j + s_k + 2y_{jk})}{s_k^2 + (1 + y_{jk}(y_{jk} + s_k))(1 + (y_{jk} + b_j)(y_{jk} + b_j + s_k))} \right) \zeta_j \right] \tag{A.1.21}$$

In Ch.6 we collect these equations and then utilise them in calculating $P(t)$ in various regions of the (α, T)-phase space.

A.2 The line $\alpha = \frac{1}{2}$

For the special case of $\alpha = \frac{1}{2}$, our collection of integrals in $K_n(t)$ are products of polynomials, indeed for $T \neq 0$ they are hyperbolic functions of the variables t_i, as such we are able to evaluate $P(t)$ to lowest order $\frac{\Delta}{\omega_c}$ simply by brute force.

We will initially consider our alternate set of equations (6.1.5) - (6.1.11) from Ch.6, and consider the case of zero temperature. This allows us to set $g(t)$ equal to unity, since

$$\lim_{x \to 0} x \left[\sinh(x)\right]^{-1} = 1 \tag{A.2.1}$$

This also means,

$$M_{jk}^{(\zeta)} = \left[\frac{g(y_{jk} + b_j + b_k + s_k)g(y_{jk} + s_k)}{g(y_{jk} + b_j + s_k)g(y_{jk} + b_k + s_k)}\right]^{\zeta_j \zeta_k} = 1 \tag{A.2.2}$$

We recall that we are limiting our attention to "interesting times" which are large compared to ω_c^{-1}, as such in the dimensionless units being used the regions over the times t_i is large compared to unity.

Rather than immediately try to find a general formula, let us consider first, the lowest three coefficients $K_n(t)$ in $P(t)$. $K_0(t)$ means that there are no blips which means we can trivially demonstrate

$$K_0(t) = 1 \tag{A.2.3}$$

Next for $K_1(t)$, we see $b_j \neq 0$, $\forall j \neq 1$. Therefore

$$F_1 = (1 + b_1^2)^{-1} \tag{A.2.4}$$

We also clearly see that $F_2 = 1$ since with only one blip there can be no interblip interactions. We now consider X_{j0} which gives us

$$X_{j0} = \tan^{-1}(t_{2j} - t_1) + \tan^{-1}(t_{2j-1} - t_0) - \tan^{-1}(t_{2j} - t_0) - \tan^{-1}(t_{2j-1} - t_1) \tag{A.2.5}$$

which when we take $t_0 \to -\infty$ we are left with

$$X_{j0} = \tan^{-1}(y_{jo} + b_j) - \tan^{-1}(y_{j0}) = \tan^{-1}\left(\frac{b_j}{1 + y_{j0}(y_{j0} + b_j)}\right) \tag{A.2.6}$$

So we are considering X_{10} which is $\tan^{-1}\left(\frac{b_1}{1 + y_{10}(y_{10} + b_1)}\right)$, which simplifies to $\tan^{-1}(b_1)$ since $y_{j,j-1} = 0$. As such F_3 is reduced to

$$F_3 = \cos\left[2\alpha \tan^{-1}(b_1)\zeta_1\right] \tag{A.2.7}$$

and since we expect the blip to be small compared to unity we set F_3 approximately equal to 1. This leaves

$$K_1(t) = \int_0^t dt_1 \int_0^{t_2} dt_1 (1 + b_1^2)^{-1} \tag{A.2.8}$$

making the substitution $x = t_2 - t_1$ then we finish with

$$-\int_0^t dt_2 \int_{t_2}^0 dx \frac{1}{1 + x^2} = \int_0^t dt_2 \tan^{-1}(t_2) = t \ \tan^{-1}(t) - \frac{1}{2}\ln(1 + t^2) \tag{A.2.9}$$

Finally, consider $K_2(t)$ where we now use our alternative representation with $g(\cdot) = M(\cdot) = 1$, which leaves us with

$$\frac{1}{2}\prod_{j=1}^2 \frac{[1 + y_{j0}(y_{j0} + b_j) + i\eta_0\zeta_1\zeta_j b_j]}{1 + b_j^2} \prod_{k=1}^{j-1}([D_{jk} + i\eta_k\zeta_j\zeta_{k+1}E_{jk}]G_{jk}^{(\zeta)}) \tag{A.2.10}$$

to evaluate this we note as before $y_{10} = 0$, and $y_{20} = s_1 + b_1$ which when substituted gives us,

$$\frac{[1 + (s_1 + b_1)(s_1 + b_1 + b_2) + i\zeta_1\zeta_2 b_2]}{(1 + b_1^2)(1 + b_2^2)}[1 + i\eta_0 b_1](D_{21} + i\eta_1 E_{21})G_{21}^{(\zeta)} \tag{A.2.11}$$

where the terms

$$D_{21} = [1 + y_{21}(y_{21} + s_1)][1 + (y_{21} + b_2)(y_{21} + b_2 + s_1)] + s_1^2 \tag{A.2.12}$$

$$E_{21} = b_2 s_1(b_2 + s_1 + 2y_{21}) \tag{A.2.13}$$

$$G_{21}^{(\zeta)} = \left\{[1 + (y_{21} + s_1)^2][1 + (y_{21} + b_2 + b_1 + s_1)^2]\right\}^{-1} \qquad \text{if} \qquad \zeta_1 = \zeta_2$$
$$= \left\{[1 + (y_{21} + b_2 + s_1)^2][1 + (y_{21} + b_1 + s_1)^2]\right\}^{-1} \qquad \text{if} \qquad \zeta_1 = -\zeta_2 \tag{A.2.14}$$

since $y_{j,j-1} = 0$, we can write after summing over $\eta_1 = \pm 1$,

$$D_{21} + i\eta_1 E_{21} = (1 + 0)(1 + b_2(b_2 + s_1)) + s_1^2 \tag{A.2.15}$$

which substituting all this back in, gives

$$(1 + ib_1)\frac{1 + b_2(b_2 + s_1) + s_1^2}{(1 + b_1^2)(1 + b_2^2)}\left[\frac{1 + (s_1 + b_1)(s_1 + b_1 + b_2) - ib_2}{[1 + (b_2 + s_1)^2][1 + (b_1 + s_1)^2]} + \frac{1 + (s_1 + b_1)(s_1 + b_1 + b_2) + ib_2}{[1 + s_1^2][1 + (b_1 + b_2 + s_1)^2]}\right] \tag{A.2.16}$$

77

which can be rewritten by multiplying the first factor through by those in large parentheses, giving us the integrand of our equation as

$$\frac{1 + b_2(b_2 + s_1) + s_1^2}{(1 + b_1^2)(1 + b_2^2)} \left[\frac{1 + (s_1 + b_1)(s_1 + b_1 + b_2) + b_1 b_2}{[1 + (b_2 + s_1)^2][1 + (b_1 + s_1)^2]} + \frac{1 + (s_1 + b_1)(s_1 + b_1 + b_2) - b_1 b_2}{[1 + s_1^2][1 + (b_1 + b_2 + s_1)^2]} \right] \tag{A.2.17}$$

where as usual $b_1 = t_2 - t_1$, $b_2 = t_4 - t_3$ and $s_1 = t_3 - t_2$ and as normal we integrate over t_1, t_2, t_3, t_4. We now approximate by remarking that for the dominant terms in this integration we expect $s_1 \gg 1$ and $b_j \lesssim 1$, which means that only those terms in the numerator and denominator proportional to s_1^4 significantly contribute which leaves,

$$I \simeq \frac{1}{2} \frac{s_1^2}{(1 + b_1^2)(1 + b_2^2)} \left[\frac{s_1^2}{(1 + s_1^2)(1 + (b_1 + b_2 + s_1)^2)} + \frac{s_1^2}{(1 + (b_1 + s_1)^2)(1 + (b_2 + s_1)^2)} \right] \simeq \frac{1}{(1 + b_1^2)(1 + b_2^2)} \tag{A.2.18}$$

Since we have rapid convergence to 0 for large values of b_i we extend the upper limit of integration to ∞, giving

$$\int_0^t dt_3 \int_0^{t_3} dt_1 \int_0^\infty \frac{db_1}{1 + b_1^2} \int_o^\infty \frac{db_2}{1 + b_2^2} = \left(\frac{\pi}{2} \right)^2 \frac{t^2}{2} \tag{A.2.19}$$

It is now clear how to proceed in the general case. Firstly through inspection of equations (6.1.6) - (6.1.10), we see that there is a set of terms with the maximum number of powers of the s_j's in the numerator and denominator of $\Phi(t_i, \zeta_i, \eta_i)$ namely $s_j^{2n(n-1)}$ (where n is the number of blips). Since the integrand of $K_n(t)$ is strictly positive, these terms will ultimately contribute a term proportional to t^n. All other terms have at least one less power of the s_j's in the numerator then in the denominator as well as one less power of each b_j, hence such terms can at most contribute a term of order $t^{n-1}(\ln t)^2$, and are thus negligible for our regime of interest, namely $t \gg 1$.

Therefore we keep only those terms with the maximum number of powers of s_j's in the numerator. As such if we rewrite E_{jk} in terms of u_{jk}, we see that we have for $k \neq j - 1$, the ability to sum over the ζ_j and the ζ_{k+1} separately which cancel out leaving $i\eta_{j-1}E_{j,j-1}$ which then drops out once we take the sum over η. We also note that by summing over j the terms $i\eta_0 \zeta_1 \zeta_j b_j$ disappears which all leaves:

$$\Phi(t_i, \zeta_i, \eta_i) \equiv \prod_{j=1}^n \frac{[1 + y_{j0}(y_{j0} + b_j)]}{(1 + b_j^2)} \prod_{k=1}^{j-1} [D_{jk} G_{jk}^{(\zeta)}] \tag{A.2.20}$$

Secondly, since the region which under integration emerges as dominant is that of large s_j and comparatively small b_j, we neglect the 1's and b_j's in our expressions for $G_{jk}^{(\zeta)}$. This means that the quantity $G_{jk}^{(\zeta)}$ becomes effectively independent of the ζ_j's, and if we define

$$R_{jk} \equiv \sum_{l=k+1}^{j-1} s_l \qquad (j \geq k + 2) \tag{A.2.21}$$

(so that $R_{j,j-2} = S_{j,j-1}$) this allows us to express, in our approximation, the ratio

$$\frac{D_{jk}}{G_{jk}^{(\zeta)}} = \left(\frac{R_{j,k}}{R_{j,k-1}} \right)^2 \tag{A.2.22}$$

which can be shown if we expand numerator and denominator while keeping only those parts proportional to s_k^2 or y_{jk}^2, to be

$$\frac{y_{jk}^2}{(y_{jk} + s_k)^2} \tag{A.2.23}$$

whereby the result follows simply by noting $y_{jk} = \sum_{l=k+1}^{j-1}(b_l + s_l) \simeq \sum_{l=k+1}^{j-1} s_l = R_{jk}$. Which we write as

$$F_n\{t_i\} = \prod_{j=1}^n \left[\frac{1}{1 + b_j^2} \cdot \frac{R_{j0}^2}{S_{j-1}^2} \prod_{k=1}^{j-1} \left[\frac{R_{jk}}{R_{j,k-1}} \right]^2 \right] = \prod_{j=1}^n \left[\frac{1}{1 + b_j^2} \right] \tag{A.2.24}$$

which is precisely the result we would have been attained if we had simply made the Non-Interacting Blip approximation from the outset. What the work in this section has done is demonstrate that the relative corrections to each of the $K_n(t)$ neglected in this approximation is rigorously of order at most $t^{-1}(\ln(t))^2$.

Finally, by restoring the units of time and extending the upper limits of integration as before, we reach the conclusion

$$K_n(t) = 2^{-n} \sum_{\{\zeta_j\}} \int_0^t dt_{2n} \dots \int_o^{t_2} dt_1 F_n\{t_i\}$$

$$= \int_0^t dt_2 n \int_0^\infty db_n \frac{1}{1 + b_n^2} \dots \int_0^\infty db_1 \frac{1}{1 + b_1^2}$$

$$= \frac{1}{n!} \left(\frac{\pi}{2} \right)^n (\omega_c t)^n \tag{A.2.25}$$

Where in the last line we have restored the units of time. Thus we can now write,

$$K_n(t) = \left(\frac{\pi}{2}\right)^n \frac{(\omega_c t)^n}{n!} \left[1 + O((\omega_c t)^{-1}(\ln(\omega_c t))^2)\right] \tag{A.2.26}$$

As such through neglecting any correction terms, then the series for $P(t)$ can be trivially summed and yields the result. Importantly, we have here demonstrated that in our limits of interest the Non-Interacting Blip Approximation is exact, as noted in Ch.6.

A.3   T=0, $0 \leq \alpha < \frac{1}{2}$

We her try to justify the Non-Interacting Blip approximation in the region $T = 0$, $0 \leq \alpha < \frac{1}{2}$ of (α, T) phase space, by qunatifying the errors which result from our approximations. We start by introducing a dimensionless time variable defined by

$$y \equiv \Delta_{\text{eff}} t \tag{A.3.1}$$

where Δ_{eff} is called the "effective inverse time scale" and is given by

$$\Delta_{\text{eff}} \equiv [\Gamma(1 - 2\alpha)\cos(\pi\alpha)]^{\frac{1}{2(1-\alpha)}} \Delta_r \tag{A.3.2}$$

Meaning that Δ_{eff} is always of order Δ_r, even being such that for $\alpha = 0$, $\Delta_{\text{eff}} = \Delta_r$. The factor $\Gamma(1 - 2\alpha)$ is introduced here since it will become useful later. If we now make the approximations given in Chapter 6.4 we may simplify as follows

$$F_n\{t_i, \zeta_m\} = \prod_{j=1}^{n} \left[f'(b_j)\right]^{2\alpha} \left(\prod_{k=1}^{n-1}\prod_{j=k+1}^{n} \left[\frac{f'(b_j + b_k + u_{jk})f'(u_{jk})}{f'(b_j + u_{jk})f'(b_k + u_{jk})}\right]^{2\alpha\zeta_j\zeta_k}\right) \prod_{k=0}^{n-1}\cos\left[2\alpha\sum_{j=k+1}^{n}\zeta_j X_{jk}\right] \tag{A.3.3}$$

the approximations leave the second term here completely untouched so let us consider the first

$$\prod_{j=1}^{n} \left[\frac{\left(\frac{\pi t}{\beta\hbar}\right)\text{cosech}\left(\frac{\pi t}{\beta\hbar}\right)}{(1 + (\omega_c t))^{\frac{1}{2}}}\right]^{2\alpha} \simeq \prod_{j=1}^{n} \frac{1}{(1 + (\omega_c t)^2)^{\alpha}} \simeq \prod_{j=1}^{n}(\omega_c t)^{-2\alpha} \tag{A.3.4}$$

where the first equality follows since we are in the limit $T \to 0$, and the second from approximation (1). If we now consider the the third term of equation (A.3.3), then we proceed as

$$\prod_{k=0}^{n-1}\cos\left[2\alpha\sum_{j=k+1}^{n}\zeta_j X_{jk}\right] \longrightarrow \prod_{k=0}^{n-1}\cos\left[2\alpha\zeta_{k+1}X_{k+1,k}\right] = \prod_{k=0}^{n-1}\cos\left[\pi\alpha\zeta_{k+1}\right] \tag{A.3.5}$$

Where here the first equality comes from applying approximation (2) and the second equality from approximation (3). We now take the sum over $\zeta_{k+1} = \pm 1$ which (since cosine is a symmetric function) leaves $[\cos(\pi\alpha)]^n$ with a prefactor from the sum. When we substitute these changes back into equation (A.3.3) we are left with

$$P(t) = \sum_{n=0}^{\infty}(-1)^n \Delta^{2n} K_n(t) \tag{A.3.6}$$

$$K_n(t) = 2^{-n}\sum_{\{\zeta_m=\pm 1\}}\int_0^t dt_{2n}\int_0^{t_{2n}}dt_{2n-1}...\int_0^{t_2}dt_1 F_n\{t_i, \zeta_m\} \tag{A.3.7}$$

$$F_n\{t_i, \zeta_m\} = \cos^n(\pi\alpha)\prod_{j=1}^{n}[\omega_c(t_{2j} - t_{2j-1})]^{-2\alpha}\prod_{k=1}^{n-1}\prod_{j=k+1}^{n}\left[\frac{(t_{2j} - t_{2k})(t_{2j-1} - t_{2k-1})}{(t_{2j} - t_{2k-1})(t_{2j-1} - t_{2k})}\right]^{2\alpha\zeta_j\zeta_k} \tag{A.3.8}$$

We wish to rewrite this in terms of our new variable y to obtain different expressions. In order that we might do this we define $z_i = \frac{t_i}{t}$ which sends $dt_i \to t dz_i$ which along with $[\omega_c t(z_{2i} - z_{2i-1})]^{-2\alpha}$ gives a factor $t^{2n(1-\alpha)}\omega_c^{2n\alpha}$ adding the terms $\cos^n(\pi\alpha)$ and Δ^{2n} gives the coefficient

$$y^{2n(1-\alpha)}[\Gamma(1 - 2\alpha)]^{-n}\Delta^{2n}\Delta_r^{-2n(1-\alpha)}\omega_c^{2n\alpha} \tag{A.3.9}$$

considering these final three terms we see they cancel out. Then after substituting z_i's for t_i's throughout, allows us to write

$$P(t) = P_r(y) = \sum_{n=1}^{\infty}(-1)^n \tilde{K}_n(\alpha)y^{2n(1-\alpha)} \tag{A.3.10}$$

$$\tilde{K}_n(\alpha) = [2\Gamma(1-2\alpha)]^{-n} \int_0^1 dz_{2n} \int_0^{z_{2n}} dz_{2n-1}... \int_0^{z_2} dz_1 \prod_{j=1}^n (z_{2j} - z_{2j-1})^{-2\alpha}$$

$$\times \sum_{\{\zeta_j = \pm 1\}} \prod_{k=1}^{n-1} \prod_{j=k+1}^n \left[\frac{(z_{2j} - z_{2k})(z_{2j-1} - z_{2k-1})}{(z_{2j} - z_{2k-1})(z_{2j-1} z_{2k})} \right]^{2\alpha \zeta_j \zeta_k} \tag{A.3.11}$$

Here we should emphasize that, for $\alpha < \frac{1}{2}$ and in the limit $\frac{\Delta}{\omega_c} \to 0$ this result is rigorous rather than (as earlier) a result of making the Non-Interacting Blip approximation. This therefore allows us to reduce our problem to one of calculating $\tilde{K}_n(\alpha)$ and the resulting series for $P_r(y)$.

Suppose first that we set the term in equation (A.3.11) contained within the large parentheses equal to one everywhere, that is, we ignore interblip interactions. Then if we call the resulting sum $P_r^{(0)}(y)$ and in turn $\tilde{K}_n^{(0)}(y)$, we are left with the expression,

$$[\Gamma(1-2\alpha)]^{-n} \int_0^1 dz_{2n} \int_0^{z_{2n}} dz_{2n-1}... \int_0^{z_2} dz_1 \prod_{j=1}^n (z_{2j} - z_{2j-1})^{-2\alpha} \tag{A.3.12}$$

We begin by changing our variables, defining $t_{2j-1} = \frac{z_{2j-1}}{z_{2j}}$ which means $dz_{2j-1} \to z_{2j} dt_{2j-1}$ we rewrite our equations as

$$= [\Gamma(1-2\alpha)]^{-n} \int_0^1 dz_{2n} \int_0^1 dt_{2n-1} \int_0^{z_{2n-1}} dz_{2n-2}... \int_0^{z_3} dz_2 \int_0^1 dt_1 \prod_{j=1}^n z_{2j} (z_{2j} - z_{2j-1})^{-2\alpha}$$

$$= [\Gamma(1-2\alpha)]^{-n} \int_0^1 dz_{2n} \int_0^1 dt_{2n-1} \int_o^{z_{2n-1}} dz_{2n-2}... \int_0^{z_3} dz_2 \int_0^1 dt_1 \prod_{j=1}^n \frac{z_{2j}^{1-2\alpha}}{(1-t_{2j-1})^{2\alpha}} \tag{A.3.13}$$

let us now start by considering the first two integrals over t_1 and z_2. Prior to this we note the definition of the so-called β-function

$$\beta(x,y) = \int_0^1 t^{x-1}(1-t)^{y-1} dt \tag{A.3.14}$$

using this we can evaluate the integral

$$\int_0^{z_3} dz_2 \int_0^1 dt_1 \frac{z_2^{1-2\alpha}}{(1-t_1)^{2\alpha}} = \beta(1, 1-2\alpha)(2-2\alpha)^{-1} z_3^{2-2\alpha} \tag{A.3.15}$$

If we substitute this into the next two integrals over t_3 and z_4, then we have

$$= \int_0^{z_5} dz_4 \int_0^1 dt_3 \frac{z_4^{1-2\alpha} z_3^{2-2\alpha}}{(1-t_3)^{2\alpha}} \beta(1, 1-2\alpha)(2-2\alpha)^{-1}$$

$$= \int_0^{z_5} dz_4 \int_0^1 \frac{z_4^{3-4\alpha} t_3^{2-2\alpha}}{(1-t_3)^{2\alpha}} dt_3 \beta(1, 1-2\alpha)(2-2\alpha)^{-1}$$

$$= \beta(3-2\alpha, 1-2\alpha)\beta(1, 1-2\alpha)(2-2\alpha)^{-1}(4-4\alpha)^{-1} z_5^{4-4\alpha} \tag{A.3.16}$$

It is clear from this that, if we inductively carry on the process, we will be able to rewrite equation (A.3.12) as

$$(\Gamma(1-2\alpha))^{-n} \prod_{j=1}^n [(2-2\alpha)j]^{-1} \beta(1 + (j-1)(2-2\alpha), 1-2\alpha) \tag{A.3.17}$$

We now use the standard relation between the Γ-function and the β-function, namely $\Gamma(x)\Gamma(y) = \beta(x+y)\Gamma(x+y)$, substituting this in we obtain,

$$(\Gamma(1-2\alpha))^{-n} \prod_{j=1}^n [(2-2\alpha)j]^{-1} \frac{\Gamma(1-2\alpha)\Gamma(1 + (j-1)(2-2\alpha))}{\Gamma(2-2\alpha + (j-1)(2-2\alpha))} \tag{A.3.18}$$

where the denominator can be written as $\Gamma[j(2-2\alpha)]$ which when multiplied by $(2-2\alpha)j$ gives (using the fact that $z\Gamma(z) = \Gamma(z+1)$)

$$(\Gamma(1-2\alpha))^{-n} \prod_{j=1}^n \frac{\Gamma(1-2\alpha)\Gamma(1 + (j-1)(2-2\alpha))}{\Gamma(1 + j(2-2\alpha))} \tag{A.3.19}$$

Now, the product of $\Gamma(1-2\alpha)$'s cancels with the prefactor $[\Gamma(1-2\alpha)]^{-n}$. We also use the fact that each denominator cancels with the subsequent numerator apart from the first and last, leaving

$$\Gamma(1)\Gamma^{-1}(1 + n(2-2\alpha)) \tag{A.3.20}$$

and since $\Gamma(1) = 1$, we have our result that

$$\tilde{K}_n^{(0)}(y) = \Gamma^{-1}\left[2n(1-\alpha)+1\right] \tag{A.3.21}$$

the series for $P_r^{(0)}(y)$ thus reduces to

$$\sum_{n=0}^{\infty}(-1)^n y^{2n(1-\alpha)}\Gamma^{-1}\left[2n(1-\alpha)+1\right] \tag{A.3.22}$$

which can be evaluated in several ways the most simple of which is by introducing the Mittag-Leffler function (p.206 [12]). If we express the series in terms of the variable $-y^{2n(1-\alpha)}$ then by use of the Mittag-Leffler function (as done by [15]), which is defined as

$$E_\alpha(z) \equiv \sum_{k=0}^{\infty}\frac{z^k}{\Gamma(\alpha k+1)} \tag{A.3.23}$$

which in our case leaves us with $E_{2(1-\alpha)}(-y^{2(1-\alpha)})$. This function is particularly complex and lengthy to evaluate and therefore we merely state the result, which is

$$P_r^{(0)}(y) = P_{\text{coh}}(y) + P_{\text{inc}}(y) \equiv \psi(y) \tag{A.3.24}$$

$$P_{\text{coh}} \equiv \frac{1}{1-\alpha}\cos\left\{\left[\cos\left(\frac{\pi}{2}\frac{\alpha}{1-\alpha}\right)\right]y\right\}exp\left\{-\left[\sin\left(\frac{\pi}{2}\frac{\alpha}{1-\alpha}\right)\right]y\right\} \tag{A.3.25}$$

$$P_{\text{inc}} \equiv -\frac{\sin(2\pi\alpha)}{\pi}\int_0^{\infty}dz\frac{z^{2\alpha-1}e^{-zy}}{z^2+2z^{2\alpha}\cos(2\pi\alpha)+z^{4\alpha-2}} \tag{A.3.26}$$

We briefly make one remark concerning these equations. The Quality factor [4] of the coherent oscillations to be found in equation (A.3.25), is independent of the timescale Δ_{eff} and is defined as

$$Q = 2\pi \times \frac{\text{Energy Stored}}{\text{Energy Dissipated per Cycle}} = \frac{\cos\left(\frac{\pi}{2}\frac{\alpha}{1-\alpha}\right)y}{\sin\left(\frac{\pi}{2}\frac{\alpha}{1-\alpha}\right)y} = \cot\left(\frac{\pi}{2}\frac{\alpha}{1-\alpha}\right) \tag{A.3.27}$$

as such it is clear that in the limit $\alpha \to 0$ the system is completely undamped, in contrast to at $\alpha = \frac{1}{2}$ where the system is overdamped, where we interpreted this value briefly in Ch.6.

We now turn to the rather delicate question regarding the corrections to the approximation $\psi(y)$ for $P_r(y)$, introduced by the interblip correlations, that is, the second factor in the integrand of eqrefintegralexpansion

$$\sum_{\{\zeta_j=\pm\}}\prod_{k=1}^{n-1}\prod_{j=k+1}^{n}\left[\frac{(z_{2j}-z_{2k})(z_{2j-1}-z_{2k-1})}{(z_{2j}-z_{2k-1})(z_{2j-1}-z_{2k})}\right]^{2\alpha\zeta_j\zeta_k} \tag{A.3.28}$$

It is clear that the difference between $P_r(y)$ and $\psi(y)$ disappears in the limit $\alpha \to 0$ (we later show it goes as $O(\alpha^2)$). Thus we turn our attention to $\alpha \to \frac{1}{2}$, initially considering only a single term (j,k) in the product as well as choosing values for $\zeta_j\zeta_k$. We redefine several terms so that

$$b_j \equiv z_{2j}-z_{2j-1} \qquad\qquad s_k \equiv z_{2k+1}-z_{2k} \qquad\qquad u_{jk} \equiv z_{2j-1}-z_{2k} \tag{A.3.29}$$

and having noted that $U_{j,j-1} = s_{j-1}$ we rewrite (A.3.28) with these definitions as follows

$$\left[\frac{(z_{2j}-z_{2k})(z_{2j-1}-z_{2k-1})}{(z_{2j}-z_{2k-1})(z_{2j-1}-z_{2k})}\right]^{2\alpha\zeta_k\zeta_k} = \left[\frac{(z_{2k}-z_{2k-1}+z_{2k-1}-z_{2k})(z_{2j-1}-z_{2k}+z_{2k}-z_{2k-1})}{(z_{2j}-z_{2k-1})(z_{2j-1}-z_{2k})}\right]^{2\alpha\zeta_j\zeta_k}$$

$$= \left[1+\frac{(z_{2k}-z_{2k-1})(z_{2j}-z_{2j-1})}{(z_{2j}-z_{2k-1})(z_{2j-1}-z_{2k})}\right]^{2\alpha\zeta_j\zeta_k} \tag{A.3.30}$$

which we finally rewrite in terms of (A.3.29) as

$$\left[1+\frac{b_jb_k}{u_{jk}(u_{jk}+b_j+b_k)}\right]^{2\alpha\zeta_j\zeta_k} \tag{A.3.31}$$

In the integrand of (A.3.11) this multiplies factors such as $b_j^{-2\alpha}$ and $b_k^{-2\alpha}$. Based on our phase-space discussions at the start of this subsection and now with b_j and s_j defined with respect to z_j's, we expect a typical blip-sojourn pair to be of order n^{-1}, which means that since $u_{jk} = \sum_{l=k+1}^{j-1}(b_l+s_l)$ then this means $u_{jk} \sim (j-k-1)n^{-1}$ for dominant contributions. Alternatively, if we were to neglect the correlations, then for α near $\frac{1}{2}$, the principal factor comes from where the factor $b_j^{-2\alpha}$

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[4]Q factor or Quality factor is a dimensionless parameter which encodes to what extent an oscillator or resonator is undamped

is largest, that is for $b_k \ll 1$. As such we will use that the primary contributions will be for blips with lengths $\sim (1 - 2\alpha)n^{-1}$. Therefore, the second term in the large parentheses of equation (A.3.31) will typically be of order,

$$\left[\frac{(1 - 2\alpha)}{(j - k - 1)} \right]^2 \tag{A.3.32}$$

The nearest-neighbour pairs (where $j = k - 1$), clearly require individual consideration. In such a case, if $u_{jk} = s_k$ is small then the correction to unity can be sizeable. However by considering (A.3.31) then

$$\left[1 + \frac{b_j b_k}{u_{jk}(u_{jk} + b_j + b_k)} \right]^{2\alpha \zeta_j \zeta_k} \sim \left[1 + \frac{(1 - 2\alpha)^2}{s_k(2 - 4\alpha + s_k)} \right]^{2\alpha \zeta_j \zeta_k} \sim \left[\frac{s_k + \frac{1}{2}(1 - 2\alpha)}{s_k} \right]^{2\alpha \zeta_j \zeta_k} \tag{A.3.33}$$

which is clearly a negligible correction if $\zeta_j = -\zeta_k$ since s_k is small, if $\zeta_j = +\zeta_k$ then we note that each introduction of a correction term cancels two terms, namely $b_j^{-2\alpha}$ and $b_k^{-2\alpha}$, which would otherwise give a factor $(1 - 2\alpha)$. As such we expect that each correction yields a contribution which is at least $(1 - 2\alpha)$ times the leading contribution, (where we set the large parentheses equal to one). As such we conjecture that in the limit $\alpha \to \frac{1}{2}$, $P_r^{(0)}(y) = \psi(y)$ is valid up to order $(1 - 2\alpha)$ and any correction for nearest-neighbour interblip correlations is valid up to order $(1 - 2\alpha)^2$.

We next show more rigorously that in the limit $\alpha \to 0$ the corrections are of order $O(\alpha^2)$ by deriving an upper limit to each $\tilde{K}_n$ from all interblip correlations. we also prove our above conjecture, that in the limit $\alpha \to \frac{1}{2}$ corrections to $\tilde{K}_n^{(0)}(y)$ will be of order $(1 - 2\alpha)$, as well as the claim that nearest-neighbour corrections are valid up to order $(1 - 2\alpha)^2$. Before this we briefly remark that none of these arguments rigorously demonstrate that $P_r^{(1)}(y)$ accurately approximates $P_r(y)$, $\forall y$ however large. In particular the relative error $\tilde{K}_n(\alpha)$ could be important for large y since $\tilde{K}_n(\alpha)$ grows with n. What these arguments do demonstrate is that for any finite value of y it is possible to choose an α sufficiently close to 0 that the corrections are negligible, as well as indicating that a very similar statement holds for α near $\frac{1}{2}$. Finally the argument indicates that for (at least) the first few cycles $P_r^{(1)}(y)$ is a very good approximation for $0 \leq \alpha < \frac{1}{2}$, this noted we continue.

Here we closely follow the work in Appendix D.2 of [3], with a small amount of material emitted or expanded upon to better suit our purpose. We firstly introduce the ratio,

$$r_n(\alpha) = \frac{\tilde{K}_n(\alpha)}{\tilde{K}_n^{(0)}(\alpha)} \tag{A.3.34}$$

where $\tilde{K}_n^{(0)}(\alpha)$ is the value obtained by neglecting the interblip factor as before, namely $\Gamma^{-1}[2n(1 - \alpha) + 1]$. We shall show that:

1. $\tilde{K}_n(\alpha) - \tilde{K}_n^{(0)}(\alpha) = O(\alpha^2)$ as $\alpha \to 0$.

2. $1 < r_n(\alpha) \leq [R(\alpha)]^{n-1}$ where $R(\alpha)$ is a finite n-independent number, for all values of $\alpha \, \epsilon \, (0, \frac{1}{2})$.

3. $r_n(\alpha) - 1$ vanishes as $(1 - 2\alpha)$ as $\alpha \to \frac{1}{2}$, and further that corrections to this through non-nearest-neighbour interactions vanish in the same limit as $(1 - 2\alpha)^2$.

Although there is not a single argument which demonstrates all 3 points, the separate arguments are not overly complex.

We may trivially rewrite equation (A.3.11) for $\tilde{K}_n(\alpha)$ as

$$\tilde{K}_n(\alpha) = [\Gamma(1 - 2\alpha)]^{-n} \int_0^1 dz_n \int_0^{z_{2n}} dz_{2n-1} ... \int_0^{z_2} dz_1 \prod_{j=1}^n (z_{2j} - z_{2j-1})^{-2\alpha} \Lambda_n \{z_m\} \tag{A.3.35}$$

where we have replaced the interblip correlation function by Λ_n such that

$$\Lambda_n \{z_m\} \equiv 2^{-n} \sum_{\{\zeta_j = \pm 1\}} \prod_{k=1}^{n-1} \prod_{j=k+1}^n [P_{jk} \{z_m\}]^{2\alpha \zeta_j \zeta_k} \tag{A.3.36}$$

$$P_{jk} \{z_m\} \equiv \frac{(b_j + u_{jk})(b_k + u_{jk})}{(b_j + b_k + u_{jk})u_{jk}} \tag{A.3.37}$$

It is useful to transform equation (A.3.35) as follows, we replace the upper limit of our final integration with z then Laplace transform the resulting function with respect to z. If we alter the order of integration it becomes apparent that the Laplace transform is proportional simply to a power of the transform variable, this allows easy inversion. When we return to $z = 1$ we are left with

$$r_n(\alpha) = [\Gamma(1 - 2\alpha)]^{-n} \int_0^\infty db_1 \int_0^\infty ds_1 ... \int_0^\infty db_n \int_0^\infty ds_n \, exp \left[-\sum_{j=1}^n (s_j + b_j) \right] \prod_{j=1}^n b_j^{-2\alpha} \Lambda_n \tag{A.3.38}$$

where Λ_n continues to be defined as above.

From here we may establish property (1) by expanding (A.3.36) in powers of α

$$[P_{jk}\{z_m\}]^{2\alpha\zeta_j\zeta_k} = exp\{2\alpha\zeta_k\zeta_j\ln(P_{jk})\} \tag{A.3.39}$$

which if we use the Taylor series expansion for 'exp' leaves us with,

$$\Lambda_n = 2^{-n}\sum_{\{\zeta_j=\pm1\}}\prod_{k=1}^{n-1}\prod_{j=k+1}^{n}[1 + 2\alpha\zeta_k\zeta_k\ln(P_{jk}) + 2\alpha^2(\ln(P_{jk}))^2 + O(\alpha^3)] \tag{A.3.40}$$

when we sum over the ζ_j we notice the term proportional to α (and indeed all odd powers of α) cancels out, leaving only corrections of $O(\alpha^2)$.

With regard to property (2), we may establish the lower bound by seeing that our quantities are not equal to one (by the corrections), as well as being positive. As such we have

$$(D_{jk} - 1)^2 > 0 \Rightarrow D_{jk} + D_{jk}^{-1} > 2 \tag{A.3.41}$$

Therefore by setting $D_{jk} = P_{jk}^{2\alpha}$ and seeing that the effect of $\sum_{\{\zeta_j=\pm1\}}$ is to give it the form of the left hand side of the second inequality the rest follows by multiplication by 2^{-n} and the products. Therefore we establish a lower bound of unity. This in turn gives a lower bound of one on $r_n(\alpha)$ since,

$$r_n(\alpha) = [\Gamma(1 - 2\alpha)]^{-n}\int_0^\infty db_1\int_0^\infty ds_1...\int_0^\infty db_n\int_0^\infty ds_n\, exp\left[-\sum_{l=1}^{n}(s_l + b_l)\right]\prod_{j=1}^{n}b_j^{-2\alpha}$$

$$= \int_0^\infty ds_1...\int_0^\infty ds_n\, exp\left[\sum_{l=1}^{n}s_l\right] = 1 \tag{A.3.42}$$

To obtain the upper bound on $r_n(\alpha)$, we define the quantity

$$H_k = \prod_{j=k+1}^{n}P_{jk} \tag{A.3.43}$$

and since (note difference between P_{jk} and $P_{jk}\{z_m\}$),

$$P_{jk} = 1 + \left[\frac{b_jb_k}{u_{jk}(b_j + b_k + u_{jk})}\right] \geq 1$$

$$\Rightarrow \Lambda_n \leq \prod_{k=1}^{n-1}H_k^{2\alpha} \tag{A.3.44}$$

we now define $Y_j \equiv b_j + s_j$, to obtain

$$\left(\frac{b_j + u_{jk}}{b_j + b_k + u_{jk}}\right) \leq \left(\frac{Y_j + u_{jk}}{Y_j + b_j + u_{jk}}\right) \tag{A.3.45}$$

since $b_k > 0$. As such,

$$H_{jk} \leq \prod_{j=k+1}^{n}\left[\frac{(Y_{jk} + u_{jk})(b_j + u_{jk})}{u_{jk}(Y_j + b_k + u_{jk})}\right] \tag{A.3.46}$$

On the right hand side we have constructed this product so that $Y_j + u_{jk} = u_{j+1,k}$ so that each term cancels two factors (one in the numerator and one in the denominator) with the term succeeding it. As a result of this we are left with

$$H_k \leq \frac{b_k + s_k}{s_k}\cdot\frac{Y_n + u_{n,k+1}}{Y_n + b_k + u_{n,k+1}} \leq \frac{b_k + s_k}{s_k} \tag{A.3.47}$$

which leaves

$$\Lambda_n \leq \prod_{k=1}^{n-1}\left(\frac{b_k + s_k}{s_k}\right)^{2\alpha} \tag{A.3.48}$$

putting this equation with the earlier equation (A.3.38) we are left with $r_n(\alpha) \leq [R(\alpha)]^{n-1}$ where we have defined $R(\alpha)$ such that,

$$R(\alpha) = [\Gamma(1 - 2\alpha)]^{-1}\int_0^\alpha\int_0^\infty e^{-(s+b)}\left[\frac{s\,b}{s+b}\right]^{2\alpha}ds\,db \tag{A.3.49}$$

83

This factor tends to $1 + 2\alpha + O(\alpha^2)$ in the limit $\alpha \to 0$, and in the limit $\alpha \to \frac{1}{2}$ it tends to 2. Thus, we give a rigorous bound quantifying the corrections to our quantity of interest, $P(t)$, from interblip correlations

$$|\delta P(t)| \leq \sum_{n=2}^{\infty} \frac{[R^{n-1}(\alpha) - 1]}{\Gamma[2n(1-\alpha) + 1]} (\Delta_{\text{eff}} t)^{2n(1-\alpha)} \tag{A.3.50}$$

as stated in [2]. As argued earlier we expect $b_j \to 0$ to give the dominant contribution as $\alpha \to \frac{1}{2}$. Although the bound on H_{jk} reduces to unity in this limit (as expected, see earlier discussion of $\alpha = \frac{1}{2}$), the behaviour in the limit $s_j \to 0$ is entirely different from that of H_{jk} itself, with the result that in our bound short sojourns and short blips are both very important. To avoid this complication we return to equation (A.3.44) and use the inequality $(1 + y)^{2\alpha} \leq 1 + y^{2\alpha}$ if $\alpha \leq \frac{1}{2}$ and $y \geq 0$, thus giving

$$P_{jk}^{2\alpha} \leq 1 + \left[\frac{b_j b_k}{u_{jk}(b_j + b_k + u_{jk})} \right]^{2\alpha} \leq 1 + \left[\frac{b_j b_k}{u_{jk}(b_j + b_k)} \right]^{2\alpha} \tag{A.3.51}$$

from which we deduce

$$\Lambda_n \leq \prod_{k=1}^{n-1} \prod_{j=k+1}^{n} \left[1 + \left[\frac{b_j b_k}{u_{jk}(b_j + b_k)} \right]^{2\alpha} \right] \tag{A.3.52}$$

As such we have the upper bound on the deviation of r_n from unity expressed as a sum of corrections from interblip interactions. This now legitimises our earlier work which gives us the result that corrections from a single nearest-neighbour term are of order $(1 - 2\alpha)$ and corrections to $P^{(1)}(t)$ are of order $(1 - 2\alpha)^2$.

Having now considered the order of corrections to $P^{(0)}(t)$, we will now consider quantitatively estimating the errors in such an approximation. To do so we follow the earlier discussion, that the nearest-neighbour correlations are most important, and as such we temporarily neglect the others. Therefore we approximate $\tilde{K}_n(\alpha)$ by $\tilde{K}_n^{(1)}(\alpha)$, where

$$\tilde{K}_n^{(1)}(\alpha) = [2\Gamma(1-2\alpha)]^{-n} \int_0^1 dz_{2n}... \int_0^{z_2} dz_1 \prod_{j=1}^{n} (z_{2j} - z_{2j-1})^{-2\alpha} \sum_{\{\zeta_k = \pm 1\}} \prod_{k=1}^{n-1} \left[\frac{(z_{2k+2} - z_{2k})(z_{2k+1} - z_{2k-1})}{(z_{2k+2} - z_{2k-1})(z_{2k+1} - z_{2k})} \right]^{2\alpha\zeta_j\zeta_k} \tag{A.3.53}$$

If we now work in units where $\Delta_{\text{eff}} = 1$, and then Laplace transform $P^{(1)}(t)$ with respect to time, we obtain

$$P^{(1)}(t) = \sum_{n=0}^{\infty} (-1)^n r_n^{(1)}(\alpha) \int e^{-\lambda t} t^{2n(1-\alpha)} dt \tag{A.3.54}$$

where the integral can be evaluated as

$$\lambda^{-2n(1-\alpha)} \int e^{-\lambda t} (\lambda t)^{2n(1-\alpha)} \frac{d(\lambda t)}{\lambda} = \lambda^{-2n(1-\alpha)-1} \Gamma[2n(1-\alpha)] \tag{A.3.55}$$

which leaves

$$P^{(1)}(t) = \sum_{n=0}^{\infty} (-1)^n \lambda^{-2n(1-\alpha)-1} r_n^{(1)}(\alpha)$$

$$r_n^{(1)}(\alpha) = [2\Gamma(1-2\alpha)]^{-n} \sum_{\{\zeta_j\}} \int_0^{\infty} db_1 \int_0^{\infty} ds_1... \int_0^{\infty} db_n \int_0^{\infty} ds_n \prod_{j=1}^{n} e^{-b_j} b_j^{-2\alpha} \prod_{j=1}^{n-1} e^{-s_j} (P_{j+1,j})^{2\alpha\zeta_j\zeta_{j+1}} \tag{A.3.56}$$

where P_{jk} is defined in equation (A.3.37), it is clear that $r_n^{(1)}(\alpha)$ is an approximation, resulting from keeping only the nearest-neighbour terms, to $r_n(\alpha)$.

We proceed according to Appendix D.3 of [3], through defining $\hat{K}$ to be a transfer operator with the effect that

$$\hat{K}[\varphi(b_1, \zeta_1)] = \psi(b_2, \zeta_2) \equiv [2\Gamma(1-2\alpha)]^{-1} \sum_{\{\zeta_1 = \pm 1\}} \int_0^{\infty} \int_0^{\infty} db_1 ds_1 e^{-(b_1 + s_1)} b_1^{-2\alpha} \left[\frac{(b_1 + s_1)(b_2 + s_1)}{s_1(b_1 + b_2 + s_1)} \right]^{2\alpha\zeta_1\zeta_2} \varphi(b_1, \zeta_1) \tag{A.3.57}$$

We also define a generalized inner product $\psi \cdot \varphi$ for any two functions $\psi(b, \zeta)$ and $\varphi(b, \zeta)$ in the form

$$\psi \cdot \varphi = [2\Gamma(1-2\alpha)]^{-1} \sum_{\{\zeta\}} \int_0^{\infty} e^{-b} b^{-2\alpha} \psi(b, \zeta) \varphi(b, \zeta) db \tag{A.3.58}$$

Finally defining the unit function to be $u(b, \zeta) = 1$. The reason we make these definitions is that it allows us to express our coefficient $r_n^{(1)}(\alpha)$ defined above in the compact form

$$r_n^{(1)}(\alpha) = u \cdot (\hat{K}^{n-1} u) \qquad\qquad n \geq 2 \tag{A.3.59}$$

Let us briefly explicitly demonstrate this for $n = 2$, then the generalization by induction will be obvious. So for $n = 2$

$$\hat{K} \cdot u = [2\Gamma(1-2\alpha)]^{-1} \sum_{\{\zeta_1 = \pm 1\}} \int_0^\infty db_1 \int_0^\infty ds_1 e^{-(b_1+s_1)} b_1^{-2\alpha} \left[\frac{(b_1+s_1)(b_2+s_1)}{s_1(b_1+b_2+s_1)} \right]^{2\alpha\zeta_1\zeta_2}$$

from which we use our inner product to find

$$u\hat{K} \cdot u = [2\Gamma(1-2\alpha)]^{-2} \sum_{\{\zeta_j = \pm 1\}} \int_0^\infty db_2 \int_0^\infty db_1 \int_0^\infty ds_1 e^{-(b_1+s_1+b_2)} b_1^{-2\alpha} b_2^{-2\alpha} \left[\frac{(b_1+s_1)(b_2+s_1)}{s_1(b_1+b_2+s_1)} \right]^{2\alpha\zeta_1\zeta_2}$$

which is as we require. If we defined $\hat{K}^{(0)}$ to be the identity operator, then since $u \cdot u = 1$ then such an expression holds for $n = 1$ as well.

We now intuitively define our function $\varphi(b, \zeta)$ to be either even or odd depending on whether $\varphi(b, -) = \varphi(b, +)$ or $\varphi(b, -) = -\varphi(b, +)$ respectively. It is clear when we consider equation (A.3.57) for $\hat{K}$ that these two groups remain invariant under the action of $\hat{K}$, i.e. $\hat{K}$ maps even functions to even functions, and odd functions to odd functions. This allows us to reduce $\hat{K}$ to its even subspace, by noting that u is clearly even. The resulting operator is necessarily symmetric and we denote the eigenvectors by ν_m and their corresponding eigenvalues by e_m, meaning that

$$\hat{K}\nu_m(\alpha) = e_m(\alpha)\nu_m(\alpha) \tag{A.3.60}$$

by imposing the condition of normalisation on the eigenfunctions ($\nu_m \cdot \nu_m = 1$) and label them in such a way that $e_1 \leq e_2 \leq e_3...$, then assuming such eigenfunctions form a basis for the subspace for $\hat{K}$ we can write

$$r_n^{(1)}(\alpha) = \sum_{m=1}^\infty e_m^{n-1}(u \cdot \nu_m)^2 \tag{A.3.61}$$

It is now clear that equation (A.3.56) is equivalent to another sum of functions of λ, where each function is associated to an eigenfunction of $\hat{K}$. To this end we rewrite equation (A.3.56) as follows

$$
\begin{aligned}
P_r^{(1)}(y) &= \sum_{n=0}^\infty (-1)^n \lambda^{-2n(1-\alpha)-1} r_n^{(1)}(\alpha) \\
&= \lambda^{-1} + \sum_{n=1}^\infty (-1)^n \lambda^{-2n(1-\alpha)-1} \sum_{m=1}^\infty e_m^{n-1}(u \cdot \nu_m)^2 \\
&= \lambda^{-1} + \sum_{m=1}^\infty \frac{1}{\lambda e_m}(u \cdot \nu_m)^2 \sum_{n=1}^\infty (-1)^n \lambda^{-2n(1-\alpha)} e_m^n
\end{aligned}
\tag{A.3.62}
$$

where we note that this last part is a geometric series giving

$$P_r^{(1)}(\lambda) = \lambda^{-1} + \frac{1}{\lambda e_m}(u \cdot \nu_m)^2 \frac{1}{1 + \lambda^{-2(1-\alpha)} e_m} - \frac{1}{\lambda \nu_m}(u \cdot \nu_m)^2 \tag{A.3.63}$$

we now make the definition

$$A_m(\alpha) = \frac{(u \cdot \nu_m)^2}{e_m} \tag{A.3.64}$$

To give us our final result (identical to page 81 of [3]), namely

$$P_r^{(1)}(\lambda) = \Lambda^{-1} \left[1 + \sum_m A_m \right] + \sum_m A_m (\lambda + \lambda^{2\alpha-1} e_m)^{-1} \tag{A.3.65}$$

we are now left with the task of inverting this equation to obtain our ultimate goal of $P^{(1)}(t)$. The first term leads to a constant, whereas the second term can be seen, through comparison with our earlier mention of the Mittag-Leffler function, to be a series similar to that earlier for $P^{(0)}(t)$. Since $f(\lambda) = \Delta_{\text{eff}}^{2(1-\alpha)} \lambda^{2\alpha-1}$ is the Laplace transform of the Mittag Leffler function (p.206 [12]), the only difference being that we have a different frequency for each m. Once we restore Δ_{eff} we are left with

$$P^{(1)}(t) = \sum_m A_m(\alpha)\psi(\Delta_m t) + C \tag{A.3.66}$$

$$\Delta_m = \Delta_{\text{eff}}[e_m(\alpha)]^{\frac{1}{2-2\alpha}} \tag{A.3.67}$$

$$C = 1 - \sum_m A_m \tag{A.3.68}$$

where ψ is the Mittag-Leffler function defined earlier. The constant C here is annoying since it implies $p \nrightarrow 0$ as $t \to \infty$ which we would intuitively expect to hold true. However numerical estimates do indicate that C does vanish up to the accuracy of such calculations [3].

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