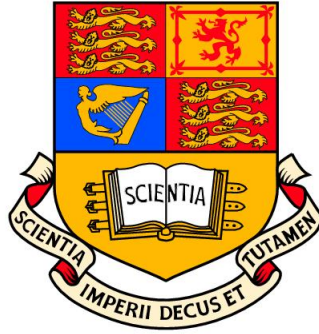


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Measurement, Decoherence and Master Equations

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Abstract

In the first part of this thesis we concern ourselves with the problem of generating pseudo-random circuits. These are a series of quantum gates chosen at random, with the overall effect of implementing unitary operations with statistical properties close to that of unitaries drawn at random with respect to the Haar measure. Such circuits have a growing number of applications in quantum-information processing, but all known algorithms require an external input of classical randomness. We suggest a scheme to implement random circuits in a weighted graph state. The input state is entangled with the weighted graph state and a random circuit is implemented by performing local measurements in one fixed basis only. A central idea in the analysis of this proposal is the average bipartite entanglement generated by the repeated application of such circuits on a large number of randomly chosen input product states. For a truly random circuit, this should agree with that obtained by applying unitaries at random chosen uniformly with respect to the Haar measure, values which can be calculated using Page's Conjecture.

Part II is largely concerned with continuous variables (CV) systems. In particular, we are interested in two descriptions. That of the class of Gaussian states, and that of systems which can be adequately described through the use of Markovian master equations. In the case of the latter, there are a number of approaches one may take in order to derive a suitable equation, all of which require some sort of approximation. These approximations can be made based on a mixture of mathematical and physical grounds. However, unfortunately it is not always clear how justified we are in making a particular choice, especially when the test system we wish to describe includes its own internal interactions. In an attempt to clarify this situation, we derive Markovian master equations for single and interacting harmonic systems under different scenarios, including strong internal coupling. By comparing the dynamics resulting from the corresponding master equations with numerical simulations of the global systems evolution, we

assess the robustness of the assumptions usually made in the process of deriving the reduced Markovian dynamics. This serves to clarify the general properties of other open quantum system scenarios subject to treatment within a Markovian approximation.

Finally, we extend the notions of the smooth min- and smooth max-entropies to the continuous variable setting. Specifically, we have provided expressions to evaluate these measures on arbitrary Gaussian states. These expressions rely only on the symplectic eigenvalues of the corresponding covariance matrix. As an application, we have considered their use as a suitable measure for detecting thermalisation.

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- [1] A. D. K. Plato, O. C. Dahlsten and M. B. Plenio, Random circuits by measurements on weighted graph states, *Phys. Rev. A* 78, 042332 (2008).
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Chapter 1

Introduction

At the very heart of quantum theory is the notion that the world is inherently uncertain. However, while this striking departure from our classical ideas may seem at first uneasy, it goes hand in hand with the many strengths these new ideas provide. Yet in its own right, randomness can itself sometimes be an advantage. Increasingly, information processing protocols are emerging which make use of the averaging properties of random quantum states and operations. Harnessing these resources on demand is very challenging, but fortunately there is an alternative. As long as we need to make use of only particular properties we can make do with a type of approximate randomness. States and operations of this type are known as pseudo-random and are typically much easier to create.

In fact, these pseudo random states can in general be produced efficiently using simple quantum gates. However all known algorithms typically require the addition of classical randomness. This extra ingredient is seemingly at odds with the inherent uncertainty present in the quantum world. It is then natural to ask whether a method exists for generating useful quantum randomness, using *just* quantum randomness. This is the topic of the first part of this thesis.

Randomness in a different form underlies much of the second part of this work.

While for the purposes of information processing, the physical system of interest is desired to be in complete isolation, in reality this is typically not the case. In many physical scenarios one has to contend with an extended system inextricably linked to our point of interest. Such a system is classed as the environment and accounting for its effect requires averaging over the statistical properties of its components. This process leads to a dynamical description based around an approximating equation called the quantum master equation.

These equations have been extensively studied in the literature, and analytic forms for single test particles exist for quite general situations (see, for example [3]). In a more realistic setting, however, the system of interest is more than just a single particle, and in general contains internal interactions along with those from the environment. With the added complexity, one has to make additional assumptions before a tractable description can be made, and in general these fall into two classes - those that assume the dominant interaction comes from the environment, and those that assume the internal couplings play the crucial role. Testing the validity of these assumptions, and knowing when one approach should be favoured over another is largely unknown.

To tackle this question, we derive example Markovian master equations for harmonic systems in the scenarios described. This allows us to then compare the dynamics resulting from their analytic treatment to a Gaussian system. These systems have the property that states are entirely described by their first and second moments, and as such large systems can be efficiently simulated. In addition, studying such systems allows us to test various assumptions usually made in the derivation of master equations, and so we can expect the conclusions to apply more generally than for our restricted class of states.

These kinds of averaging interactions also play a more fundamental role in physics. They lie at the heart of the statistical mechanics approach to thermodynamics. The aim here is to describe physical quantities in terms of aggregated properties of the microstates of a system. One often tries to link this theory to the Second Law through the entropy, and in the quantum mechanical setting the natural choice is the von Neumann entropy. However, this is by no means the

only entropy measure that exists and one could ask whether there may in fact be a more appropriate quantity on which to base the study of thermodynamics. This rests on the observation that operational interpretations of the von Neumann entropy usually assume a large number of identical and independent distributions (i.i.d), and while this is precisely the situation one expects in macroscopic systems, one could argue that for small quantum systems this need not apply. In this case we can appeal to more general entropy measures, and in particular we shall look at what are called the “min” and “max” entropies.

This thesis is structured as follows:

Chapter 2 is concerned with generating pseudo random unitary operators by means of an entirely quantum algorithm. This is done in the framework of a generalised measurement based quantum computation model, where the conventional graph state resource is extended to a weighted graph state. As a result we sacrifice computational determinism in favour of a random evolution, and as a consequence only measurements in a fixed basis are required. We begin by reviewing the notion of random unitary operators and quantum t -designs, and define our requirements for a pseudo random circuit. This is a series of quantum gates chosen at random (with unspecified bias) that have the effect of approximating uniformly random unitaries. We then define our scheme based on a weighted graph state resource, and analyse it’s performance by comparing the resulting entanglement probability distribution with that associated to the Haar measure on pure states given by “Page’s conjecture” [28]. In the appendices we present further generalisations.

Chapter 3 and **Chapter 4** introduces background material on Gaussian state and Markovian master equations. While these cannot be considered a definitive review, they contain all the material relevant for Part II of this thesis.

Chapter 5 derives Markovian master equations for single and interacting harmonic systems. Care is taken to preserve complete positivity, which in some

cases distinguishes our results from those found elsewhere in the literature. In particular, we derive our equations under different parameter regimes, including strong internal coupling and compare the obtained dynamics with those of simulated exact (Gaussian) system. In each case we assess the robustness of the assumptions usually made in the process of deriving the reduced Markovian dynamics.

Chapter 6 deals with deriving expressions for the min- and max- entropy for arbitrary Gaussian states. By proving a suitable ansatz, we also present a numerical prescription for calculating smooth entropies for multi-mode states. In some cases this allows us to provide bounds on improving the numerical efficiency, while in others we find exact analytic expressions. Using these results, we compare the min-entropy to the von Neumann entropy as a measure of equilibration, again by simulating a thermalisation process exactly using Gaussian states, and approximately using master equations from Chapter 5.

The work in **Chapter 2** was carried out along with Oscar Dahlsten and Martin Plenio. **Chapter 5** is joint work with Ángel Rivas, Susana Huelga and Martin Plenio, while **Chapter 6** contains as yet unpublished material resulting from a collaboration with Lidia del Rio, Oscar Dahlsten and Martin Plenio.

Part I

Measurement

Chapter 2

Pseudo Random Circuits

2.1 Introduction

Randomising operations have traditionally had a wide usage in information processing. In the classical setting, drawing randomly from a probability distribution has had applications in simulation, such as with Monte Carlo methods, cryptography and in many types of randomised algorithms. Surprisingly, these can often lead to speed improvements over any known deterministic approach. A prime example is that of polynomial identity testing [4]¹, where given two polynomials P and Q over a field F we wish to decide whether they are equal $P \equiv Q$. A first approach may be to simply expand the polynomials and compare terms, however this may often lead to exponentially many terms. Instead we can employ a randomised algorithm. Note that $P \equiv Q$ iff $P - Q \equiv 0$, and so for a univariate polynomial of degree n we have at most n distinct roots. Thus, if we choose an arbitrary subset $S \subseteq F$ such that $|S| \geq 2n$ then the probability of evaluating some $x \in S$ drawn at random and obtaining $(P - Q)(x) = 0$ when $P - Q \not\equiv 0$ is,

$$\Pr((P - Q)(x) = 0) \leq \frac{n}{|S|}. \quad (2.1)$$

¹Other examples include quicksort and primality testing.

In the case of quantum information processing, rather than conventional random numbers we are instead usually interested in making use of a random state, or more often a random unitary operation. However, such unitaries cannot be generated directly, but instead need to be implemented as a sequence of random elementary gates. Such a collection is known as a random circuit.

The number of applications for random circuits in quantum information processing is growing. They may be applied to hide information about input states [5], to sample state spaces [6], and to model random processes such as thermalisation [7, 8, 9, 10, 11, 12, 13] and black hole information leakage [14]. A more surprising application is in the superdense coding of quantum states [15]. Generating uniformly random operators over $U(2^N)$ is, however, exponentially hard and instead it is often sufficient to produce circuits which are identical in only a few of the relevant statistical properties. This concept can be formalised by the notion of a quantum design, which shall be discussed in the Section 2.1.2. Such pseudo-random circuits have already been efficiently implemented in an *NMR*-setup [19].

In this chapter we will propose a new implementation for such random circuits. One prepares, in advance, a highly entangled resource state called a weighted graph state. The input state is entangled with a number of qubits in the resource state and the experimenter then performs local measurements in one fixed basis only. The randomness of the measurement outcomes effectively pick the circuit, and the output state is then carried by a subset of qubits of the total system.

Such a scheme has several advantages. First, no additional classical random numbers are used in the process, so the randomness is entirely quantum. Furthermore, the measurement based approach has the benefit of being comparatively scalable and the fact that the experimenter only needs to measure in one basis throughout is a simplification and is to our knowledge at present unique to our scheme. In addition, as this is a new application of weighted graph states it may help to motivate such experiments. Recent work has independently suggested the measurement based approach for generating random circuits [20]. They were able to improve on a previously known gate model, by first translating it into the

conventional cluster state formalism. Here, however, we find that using weighted graph states is arguably more natural and simple: no classical pseudo-random numbers are required, and measurements are only performed in one basis.

We proceed as follows. Firstly background material on random circuits, measurement based quantum computation and weighted graph states is presented. We then define and analyse our proposed method. In the subsequent sections the scheme is evaluated, and finally we summarise possible experimental implementations and discuss open questions.

2.1.1 Preliminaries

To set notation, we begin with a few preliminaries. Throughout this chapter we will use interchangeably σ_k , $k = x, y, z$ and X , Y , and Z to represent the Pauli matrices, along with $\mathbb{I}$ to represent the identity operator,

$$\mathbb{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad Y = -iZX = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}. \quad (2.2)$$

Following the usual convention, the eigenstates of the Z and X operators are then,

$$\begin{aligned} Z|0\rangle &= |0\rangle, & X|+\rangle &= |+\rangle \equiv \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle), \\ Z|1\rangle &= -|1\rangle, & -X|-\rangle &= |-\rangle \equiv \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle). \end{aligned} \quad (2.3)$$

Mappings between these sets of eigenstates are generated through the Hadamard operator,

$$\begin{aligned} H|0\rangle &= |+\rangle, \\ H|1\rangle &= |-\rangle. \end{aligned} \quad (2.4)$$

Taken together, (2.3) and (2.4) then imply the following useful relations

$$HXH = Z, \quad HZH = X, \quad HYH = -Y, \quad (2.5)$$

which generalise quite naturally to rotations $U_k(\phi) = e^{-\frac{i\phi}{2}\sigma_k}$, by an angle ϕ about the k axis on the Bloch Sphere.

In addition, we shall frequently make use of the Controlled- Z gate (CZ) defined by the operation $|0\rangle\langle 0| \otimes \mathbb{I} + |1\rangle\langle 1| \otimes Z$. The action on the computational basis of any 2-qubit state is then given by,

$$CZ|i\rangle|j\rangle = (-1)^{ij}|i\rangle|j\rangle. \quad (2.6)$$

Where appropriate for clarity, will assign operators a subscript label to identify the states they act on.

2.1.2 Quantum t -designs

Sampling from the Haar distribution is inefficient, however it is often the case that a particular application does not require a true random operator. Instead we may make do with choosing from a collection of *pseudo-random* operators, so long as their properties are close enough to those of the uniform distribution. A common requirement is that the distribution is indistinguishable with the Haar distribution, for up to a finite number of moments. This notion is formalised by the following definitions.

State t -design

A (state) t -design is a finite ensemble of states $\{p_i, |\phi_i\rangle\}$ which are indistinguishable from the uniform probability distribution (Haar measure) over all quantum states using any test where we are given only t copies of a state from the ensemble. This notion can be formalised in the following definition [45]

2.1.1. DEFINITION. A probability distribution over quantum states $\{p_i, |\phi_i\rangle\}$ is a *quantum state t -design* if

$$\sum_i p_i (|\phi_i\rangle\langle\phi_i|)^{\otimes t} = \int_{\psi} (|\psi\rangle\langle\psi|)^{\otimes t} d\psi. \quad (2.7)$$

where the integral on the right hand side is taken over the left-invariant Haar measure on the unit sphere in $\mathbb{C}^d$.

State designs have the advantage in that they can be implemented efficiently in **polytime** [16, 18]. Alternatively, state designs can also be defined in terms of the highest order for which an arbitrary polynomial in the amplitudes of states chosen from the design and the Haar measure produce the same expectations. We define a monomial to be of degree (t_1, t_2) if it contains a term with t_1 conjugated elements and t_2 unconjugated elements, being termed *balanced* (and of degree t) if $t = t_1 = t_2$. Then a state (t, t) -design can be defined in terms of amplitudes of a state $|\phi\rangle = \sum_{j=1}^N \alpha_j |j\rangle$ as follows [45],

2.1.2. DEFINITION. A probability distribution over quantum states $\{p_i, |\phi_i\rangle\}$ is a *quantum state (t, t) -design* if for an arbitrary polynomial $p(\phi)$ of degree (t, t) in the variables $\alpha_1, \dots, \alpha_N$ and $\alpha_1^*, \dots, \alpha_N^*$,

$$\sum_i p_i p(\phi_i) = \int_{\psi} p(\psi) d\psi. \quad (2.8)$$

Definitions 2.1.1 and 2.1.2 can be shown to be equivalent ([45], Theorem 5) by noting the following. Each element in the matrix $\sum_i p_i (|\phi_i\rangle\langle\phi_i|)^{\otimes t}$ is just an expectation of a monomial in the amplitudes of a state chosen from the design, while the corresponding entry in the matrix $\int_{\psi} (|\psi\rangle\langle\psi|)^{\otimes t} d\psi$ is the expectation when the state is instead chosen from the Haar measure. If the expectations are the same for any monomial then accordingly the matrices $\sum_i p_i (|\phi_i\rangle\langle\phi_i|)^{\otimes t}$ and $\int_{\psi} (|\psi\rangle\langle\psi|)^{\otimes t} d\psi$ are equal and so Definition 2.1.2 implies Definition 2.1.1, as if it is true for all monomials, it is true for all polynomials as well. To see the converse, we note that for every balanced monomial of degree t , there is an entry

in $\int_{\psi} (|\psi\rangle\langle\psi|)^{\otimes t} d\psi$ equal to its expectation.

Unitary designs

A unitary design can in many ways be thought of as a stronger version of a state design. In the same way that applying a unitary drawn uniformly from the Haar measure to an arbitrary pure state results in a uniformly random pure state, acting on an arbitrary pure state with a unitary t -design produces a state t -design. Put another way, given t d -dimensional systems, then a unitary t -design is an ensemble of unitaries such that when one is drawn from the collection at random and applied to each of the systems the resulting state is indistinguishable from having instead applied a uniformly random unitary. We then have:

2.1.3. DEFINITION. An ensemble of unitary operators $\{p_i, U_i\}$ is a *unitary t -design* iff for all $d^t \times d^t$ matrices ρ

$$\sum_i p_i U_i^{\otimes t} \rho (U_i^\dagger)^{\otimes t} = \int_U U^{\otimes t} \rho (U^\dagger)^{\otimes t} dU. \quad (2.9)$$

Known unitary designs are inefficient to implement however efficient approximate (see below) unitary 2-designs have been proposed in the literature [17]. Just as for state designs, we can instead define a unitary t -design in terms of averages of polynomials:

2.1.4. DEFINITION. ([17]). A set of unitary operators $\{U_i\}$ is a unitary t -design if for all balanced monomials p of degree t ,

$$\sum_i p(U_i) = \int_U p(U) dU. \quad (2.10)$$

Approximate t -designs

Finally, while exact unitary designs are often inefficient to implement, an approximate t -design may be possible. These can be defined in terms of ϵ closeness to their exact counterparts:

2.1.5. DEFINITION. A probability distribution over quantum states $\{p_i, |\phi_i\rangle\}$ is an ϵ -approximate *quantum state t -design* if

$$(1 - \epsilon) \int_{\psi} (|\psi\rangle\langle\psi|)^{\otimes t} d\psi \leq \sum_i p_i (|\phi_i\rangle\langle\phi_i|)^{\otimes t} \leq (1 + \epsilon) \int_{\psi} (|\psi\rangle\langle\psi|)^{\otimes t} d\psi. \quad (2.11)$$

and analogously for unitary t -designs.

2.2 Random Circuits

In any practical implementation, random (or pseudo-random) unitary operators cannot be generated directly. Instead, they must be implemented as a sequence of simpler quantum gates. The requirements that they obey particular statistical properties imply that these in turn must be applied in a probabilistic fashion. Such a *sequence of quantum gates picked at random* is called a *random circuit*. Thus according to this definition, a simple example of a random circuit for a single qubit is the following: apply the Hadamard gate H , Pauli X or $\mathbb{I}$ each with probability $1/3$. However, in practice, we are often more interested in random circuits with the properties mentioned above, and so we include three additional conditions that such proposals should satisfy. These will serve as the basis for our later evaluation.

(i) *Unbiased sampling asymptotically*

For hiding an input state fully one requires the output states to have a flat distribution in state space, i.e. according to the unitarily invariant Haar measure P where $P(|\Psi\rangle) = P(U|\Psi\rangle)$. It is a simple but important observation that if the gates are picked from a non-universal set one would not access all states, and therefore not achieve the uniform distribution, even in the asymptotic limit. In fact it is essentially sufficient for a random circuit to consist of gates picked from a universal set of gates for it to induce the Haar measure asymptotically - see [22] for discussion.

(ii) *Good sampling in polynomial time*

Unbiased sampling of the uniform distribution to within a fixed accuracy re-

quires $\exp(N)$ elementary gates, where N is the number of qubits [22]. However for practical applications one will require the circuit to give a sufficiently good sampling in a modest, i.e. $\text{poly}(N)$ time. What merits being called a sufficiently good sampling can depend on the application. For example, in superdense coding of quantum states [15, 13, 24] one requires that the entanglement is typically maximal [25, 26, 27, 28, 31]. In fact, typically maximal entanglement may be achieved to some accuracy within $\text{poly}(N)$ elementary gates picked at random. Such schemes exist [12, 13], the results of which were recently generalised in [33].

(iii) Feasible experimental implementation

For practical applications we furthermore require a feasible experimental implementation, ideally one that is possible with current technology.

It should be noted that the unbiased sampling of property *(i)* is often included in definitions of random (and pseudo-random) circuits found elsewhere in the literature.

2.2.1 An Application: Superdense Coding

As an example, we will now demonstrate the usefulness of random unitary operators by looking at superdense coding. In particular, we will see how one can extend the case of sharing classical bits to qubits, provided of course we accept some chance of failure. First, let us recall the original scenario [29] where Alice and Bob initially share the Bell state $|\Phi^+\rangle = \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle)$, and Alice wishes to send Bob two classical bits of information. In advance, the two parties agree on an encoding for the four possible bit strings on to the operations $\mathbb{I}$, X , Y and Z . If Alice now performs one of these on the qubit she is holding, then the result is

that the total state now becomes one of the four maximally entangled Bell states,

$$\begin{aligned}
\mathbb{I} \rightarrow |\Phi^+\rangle &= \frac{1}{\sqrt{2}}(|00\rangle + |11\rangle), \\
X \rightarrow |\Psi^+\rangle &= \frac{1}{\sqrt{2}}(|10\rangle + |01\rangle), \\
Y \rightarrow -i|\Psi^-\rangle &= \frac{-i}{\sqrt{2}}(|10\rangle - |01\rangle), \\
Z \rightarrow |\Phi^-\rangle &= \frac{1}{\sqrt{2}}(|00\rangle - |11\rangle).
\end{aligned} \tag{2.12}$$

She can now send her qubit to Bob who, by performing orthogonal measurements, can detect which of the four operations Alice carried out. Thus we see, that by sharing one ebit and sending one qubit Alice has been able communicate two classical bits of information. This “doubling up” of information is known as superdense coding, and summarising one may write,

$$1\text{qubit} + 1\text{ebit} \succeq 2\text{cbits}. \tag{2.13}$$

Suppose now however, that instead of classical bits Alice wishes to communicate two qubits to Bob using the same resource. The above inequality suggests that this is in fact impossible, as if it were true then we could take these two qubits together with two additional ebits and generate four qubits. Iterating repeatedly with a sufficiently large amount of entanglement would then allow us to communicate an arbitrary amount of information by sending only one qubit. This is known to be impossible [30].

However, if Alice is willing to accept some probability of failure, then she can communicate any arbitrary state to Bob. Notice above, that by performing operations on only her portion of the state, Alice could convert between any of the maximally entangled Bell states. In fact, this is true more generally where any arbitrary maximally entangled state $|\psi\rangle$, of dimension d can be related to a fixed maximally entangled state $|\Phi_d\rangle = \frac{1}{\sqrt{d}} \sum_i |i\rangle|i\rangle$ through a local unitary operation alone [15],

$$|\psi\rangle = V(\psi) \otimes \mathbb{I} |\Phi_d\rangle, \tag{2.14}$$

where $V(\psi)$ is a unitary operator which depends on the desired state $|\psi\rangle$. If Alice had previously promised to Bob that she would send only such states, then the protocol could proceed perfectly. For an arbitrary state however, we can do *almost* as well. Rather than communicate a state $|\psi\rangle$ directly, Alice and Bob instead agree beforehand on a unitary operator U_{AB} drawn from the Haar measure on $U(2^d)$. Then the state $U_{AB}|\psi\rangle$ is very nearly always maximally entangled for large dimensions [26, 27, 28]. Alice's goal is then to share this state with Bob, by first applying the unitary $V(U_{AB}|\psi\rangle)$ to her state alone,

$$U_{AB}|\psi\rangle = V_A(U_{AB}\psi) \otimes \mathbb{I}_B|\Phi_d\rangle. \quad (2.15)$$

She then sends her part to Bob, who can then recover $|\psi\rangle$ by performing the operation $U_{AB}^\dagger$ on the combined state. We stress that while the unitary U_{AB} acts on the composite system, Alice only ever need operate on her local portion. The protocol then succeeds provided that the target encoding is in fact on to a maximally entangled state. For a detailed analysis of the success rate and communication cost see [15, 34, 35].

2.3 Measurement based quantum computation

We now review the basic features of measurement based quantum computation (MBQC). In particular, we will focus our attention on the one way quantum computation (1WQC) model of Raussendorf and Briegel [32], as the extension to our weighted graph state scheme in later sections follows in a straightforward manner. Here the central idea relies on creating, in advance, a large entangled resource state, known as a cluster or graph state (see Section 2.4). Input states are then encoded on a collection of qubits, which in turn are entangled with the resource state via Controlled-Z operations. Performing patterns of adaptive single qubit measurements on sites in the entire state coherently teleport the input state through the resource, performing part of the computation at each step. After the desired computation has been performed, the output can then be read off from

the resulting projected state on the final set of qubits.

To describe the 1WQC model, let us first consider a simple teleportation of a single qubit in state $\psi = \alpha|0\rangle + \beta|1\rangle$ on to a qubit initially prepared in the $|+\rangle$ state. The first step is to entangle the two qubits using the Controlled- Z operation, $|0\rangle\langle 0| \otimes \mathbb{I} + |1\rangle\langle 1| \otimes Z$, leading to the combined state,

$$\begin{aligned} CZ|\psi\rangle|+\rangle &= CZ_{12}H_2|\psi\rangle_1|0\rangle_2 \\ &= H_2CX_{12}(\alpha|0\rangle_1|0\rangle_2 + \beta|1\rangle_1|0\rangle_2) \\ &= \alpha|0\rangle|+\rangle + \beta|1\rangle|-\rangle, \end{aligned} \tag{2.16}$$

where we have used the relations (2.4) and the fact that a CZ gate can be converted to a $CNOT$ by passing through a Hadamard gate acting on the second qubit. The first qubit is then measured in the basis $\{|0\rangle \pm e^{i\phi}|1\rangle\}$, with the two outcomes projecting the second state into either,

$$\alpha|+\rangle \pm e^{-i\phi}\beta|-\rangle. \tag{2.17}$$

The $+1$ eigenvalue result corresponds to the state above with the $+$, while a -1 corresponds to the $-$ state. In what follows it will be convenient to introduce the notation of a measurement outcome index, $s \in \{0, 1\}$ to represent the obtained eigenvalues $(-1)^s$. Later we will extend this notation to a binary vector, S , so that we may include the outcomes of multiple concatenated measurements. Using this notation, we can then write the projected state, up to a global phase, as

$$X^s H U_z(\phi) |\psi\rangle. \tag{2.18}$$

Thus we see by teleporting our original state, we have performed the unitary transformation $X^s H U_z(\phi)$. To see how any single qubit operation can be performed, we repeat the above two qubit protocol three times, with the transformed qubit of one acting as the input state of the next. Thus the combined effect is to

implement the unitary transformation,

$$U = X^{s_3} H U_z(\phi_3) X^{s_2} H U_z(\phi_2) X^{s_1} H U_z(\phi_1). \quad (2.19)$$

Now, using the first relation in (2.5) and that $H U_z(\phi) H = U_x(\phi)$ we can write,

$$U = H Z^{s_3} U_z(\phi_3) X^{s_2} U_x(\phi_2) Z^{s_1} U_z(\phi_1). \quad (2.20)$$

Finally, noting that commuting a Pauli X (Z) through a rotation $U_z(\phi)$ ($U_x(\phi)$) introduces a minus sign in the angle, i.e. $X U_z(\phi) = U_z(-\phi) X$ etc., we can pass all the Pauli operations to the left and so the overall unitary transformation becomes,

$$U = X^{s_3} Z^{s_2} X^{s_1} H U_z((-1)^{s_2} \phi_3) U_x((-1)^{s_1} \phi_2) U_z(\phi_1). \quad (2.21)$$

We can now see that by virtue of the Euler Rotation theorem we can implement *any* single qubit rotation, provided that we impose a natural time ordering of the measurements. That is, each measurement outcome influences the choice of basis for the next measurement and so to implement an arbitrary rotation we choose the measurement angles to be $\phi_1 = \alpha$, $\phi_2 = (-1)^{s_1} \beta$ and $\phi_3 = (-1)^{s_2} \gamma$. Provided we make the appropriate choice after the previous measurement result is obtained, then the computation is deterministic. All that is left is to account for the leftover Pauli operations, which is easily done via classical post-processing. To see how such a protocol can be extended to include universal quantum computation we need only demonstrate an entangling two-qubit gate. To do this, we simply note that our resource state already includes such a gate in the form of the entangling CZ operations. Extending the 1-dimensional chain of $|+\rangle$ qubits to a 2-dimensional array gives the desired ingredients. It is worth noting that as the CZ operations commute with the relevant measurements, the entire resource state can be prepared in advance. Such a construction is known as a graph or cluster state, and any quantum computation is implemented as a pattern of adaptive measurements on each qubit, along with the classical post-processing mentioned above.

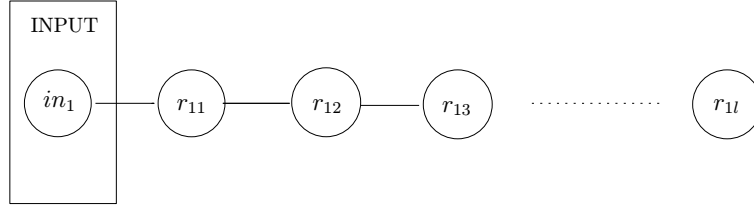


Figure 2.1: A resource state for quantum computation on a single qubit together with the input state. Circles represent qubits and the qubit (in_1) carries the input state. The figure shows the state before the measurements have been performed. Solid lines indicate CZ gates. The resource qubits are in the $|+\rangle$ state before the CZ is applied. They are labelled $r_{11}, r_{12} \dots r_{1l}$, where l signifies the length of the circuit and the first and second index are the row and column in the graph respectively.

This ability to do most of the entangling operations beforehand is one reason why the measurement based quantum computing approach is often argued to be easier to implement in experiment than the circuit model. Here one can do most of the entangling operations before the input state has been given. Since these gates are particularly difficult to do, it is desirable to be able to fail and redo them, without losing the input state. Only when this has been successfully achieved does one give the input state. This requires entangling the qubits carrying that state with those in the resource. After which, only local measurements on the system are necessary to achieve an arbitrary unitary transformation [36].

2.3.1 Random circuits in One Way Quantum Computation

Most algorithms for generating random (or pseudo-random) unitaries are based on the gate model of quantum computation. However, as the measurement based approach is also capable of universal quantum computation it follows that such algorithms can be recast in this formalism. Conceptually the simplest is that of Emerson *et al.* [19] which acts by repeatedly applying unitaries drawn at random from a set of universal gates. Such a set can be shown to generate the Haar measure asymptotically [22], regardless of the way choices are biased. However, it was also demonstrated that such a scheme is capable of generating

pseudo-random unitaries with circuits which scale in length only polynomial in the number of input qubits N .

Before outlining how this may be used in the context of 1WQC using conventional graph states, we will first briefly describe the construction of the universal set in the gate model. This requires two steps. First, we draw a set of N independent single qubit unitaries from the Haar measure on $U(2)$. These will be applied to rotate each of the N qubits on our input state. In order to guarantee that these are indeed drawn uniformly from the Haar measure, we may construct them exactly from the Hurwitz decomposition [23], using 3 random variables each. Alternatively, we may be happy with some other choice of bias², for example by using the Euler rotation theorem above. However it should be noted that regardless of our choice this step explicitly requires the addition of some form of randomness, whether classical or quantum. The next step is to entangle all nearest neighbour pairs of qubits using a fixed two-body interaction of the form,

$$U = \exp \left[i(\pi/4) Z^{j_1} \otimes Z^{j_2} \right], \quad (2.22)$$

which in essence is a CZ gate up to single qubit rotations.

The conversion to the 1WQC approach is then straightforward. Random single qubit rotations, 2.21, are implemented through three measurements with angles ϕ_1 , ϕ_2 and ϕ_3 , while the second step two qubit unitaries are provided by the CZ gates. In this case we have the additional simplification that the measurements are no longer adaptive as the Haar measure is invariant under the additional Pauli operations. The convergence rates of this scheme can in fact be improved by including a CZ gate between each nearest neighbour qubit after each measurement [20, 21] (i.e. between every qubit in the vertical rows of the cluster state). This corresponds to restricting the class of $U(2)$ operations above to $U_z(\phi)$, and results in an algorithm speed improvement by an approximate factor of 6.

²In fact, it has been shown that in some cases, a restricted set of single qubit gates can converge faster to an approximate 2-design [21, 20]. For pedagogical reasons we begin by assuming the full $U(2)$ group, however we discuss one example of the restricted case below.

2.4 Weighted graph states

There are many types of resource states one can use for measurement based quantum computation. In this section we define a type of resource state called a graph state [36]. Then we introduce a natural generalization thereof called weighted graph states, which is what we will use for our scheme.

We begin by defining a *graph*, $G = (V, E)$, as a finite non-empty point set V along with a collection $E \subset V$ of unordered pairs of points in V . We say V is the collection of the points or vertices of G and E the collection of edges. A graph is *simple* if it is undirected, and has no loops or weights. We can describe a graph by the elements of a matrix Γ_{ab} , where entries correspond to whether an edge connects vertices a and b . For unweighted graphs, $\Gamma_{ab} = 1$ for all $\{a, b\} \in E$ and zero otherwise. Such a matrix is called an adjacency matrix of the graph G , and so a simple graph can be described by a symmetric matrix, of ones and zeros, having zeros along the main diagonal.

Graphs such as these can be used to describe a family of quantum states in the following manner. We first consider each vertex as labeling a qubit in the state $|+\rangle$. Between each pair of qubits connected by an edge in the associated graph we apply a unitary operation $U_{ab}(\Gamma) = e^{-i\Gamma_{ab}\frac{\pi}{4}(I-Z_a)\otimes(I-Z_b)}$, i.e. a CZ gate. The resulting states described by this procedure are graph states, and includes the cluster state resources as special cases. Using this formulation, it is then straightforward to generalise graph states to weighted graph states (WGS), by simply relaxing the condition that edges carry no weights. Thus, the simplest definition of a weighted graph state is,

$$|\Psi_{WGS}\rangle = \left(\prod_{\{a,b\} \in E} U_{ab}(\Gamma_{ab}) \right) |+\rangle^{\otimes N}, \quad (2.23)$$

where the product is taken over all edges $\{a, b\}$ and the unitaries are now defined by $U_{ab} = e^{-i\Gamma_{ab}\frac{\pi}{4}(I-Z_a)\otimes(I-Z_b)}$, where Γ_{ab} are given by the components of the adjacency matrix of a weighted graph.

Various applications and generalisations of weighted graph states themselves

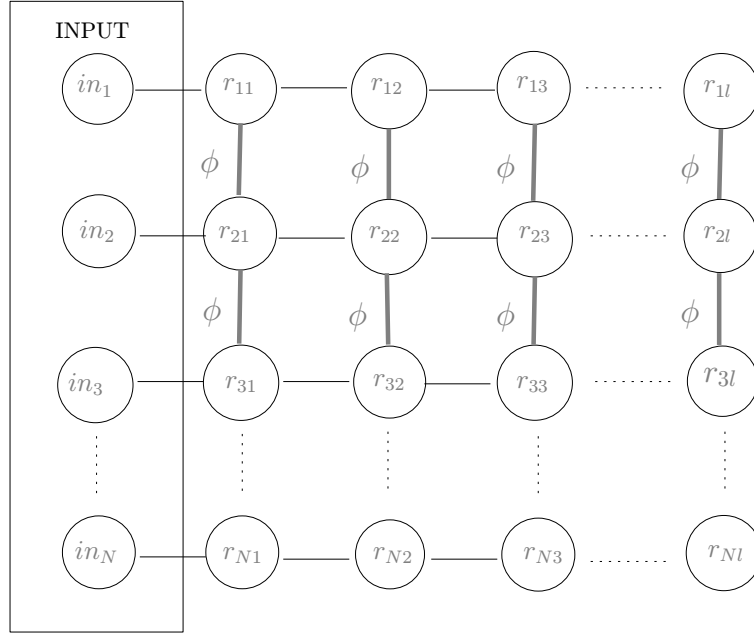


Figure 2.2: The initial weighted graph state resource used in our random circuit generation scheme prior to any measurements, together with the column of qubits carrying the input state. Circles represent qubits and the qubits $(in_1, \dots, in_N)$ carry the input state. Thin horizontal lines indicate CZ gates, while thicker vertical lines are ϕ gates, defined in equation (2.24). The resource qubits are in the $|+\rangle$ state before the CZ and ϕ gates are applied. Each lie on a vertex $a = (j, k)$ in a graph G and take the labeling r_{jk} . j is the row index which runs from 1 to N , the number of qubits in the input state. k is the column index which runs from 1 to l , the length of the circuit.

have been proposed [37, 38, 39]. For example, one can include more general initial states, additional filtering operations and local unitary operators. However, for the purposes of this thesis, the above definition captures the relevant ideas needed to extend the cluster state formalism.

2.5 Measurement based scheme

We now describe our scheme for generating random circuits, using ideas from measurement based quantum computation. The key feature in this proposal is the adoption of weighted graph states as the resource states for measurement based quantum computing. This enables us to present a simple, fixed measure-

ment algorithm which does not have the requirement of a separate classical (or quantum) random number generator. It follows closely the simplest cluster state model, with only minor variations in the non-local operations made between adjacent rows.

First, we describe the proposed scheme. Then we characterise the associated evolution of the input state. This is important for showing that the process is unitary.

The proposal is as follows. First, a planar rectangular array of $N \times l$ qubits is prepared, each initially in the state $|\psi\rangle_{r_{jk}} = |+\rangle$ with subscripts j and k labeling the row and column positions along the array, see Fig 2.2. This configuration is represented by a graph G embedded in a 2D lattice, and so a vertex, a , is described by two numbers (j, k) , and on each vertex lies a qubit r_{jk} . Between each pair of adjacent qubits on neighbouring columns we apply CZ gates, that is, $U_{r_{jk}r_{jk\pm 1}} = \text{diag}(1, 1, 1, -1)$. Between each pair of adjacent qubits on neighbouring rows we apply the controlled phase gates,

$$U(\phi_{r_{jk}r_{j\pm 1k}}) = \text{diag}(1, 1, 1, e^{-i\phi_{r_{jk}r_{j\pm 1k}}}), \quad (2.24)$$

where the parameters $\phi_{ab} = \Gamma_{ab}\frac{\pi}{4} = \phi$ for all a, b . We will refer to this as the ϕ -gate. As these operators commute, they can be carried out in parallel. The number of rows needed is determined by the number of qubits on which the random unitary will act, while the depth or length l specifies the number of iterations to be performed. Note that it will not be necessary to prepare the entire resource state to depth l initially - it may be grown as the protocol proceeds. The circuit acts on an N qubit state $|\Psi\rangle_{in}$ carried by qubits $in_1, in_2 \dots in_N$. A CZ gate is applied between each in_j and r_{j1} qubit. Then each in qubit is measured in the basis $\{|+\rangle, |-\rangle\}$. The possible outcomes are labeled by a binary vector $\vec{S}^{(k)}$ where each component $S_j^{(k)}$ takes the value $S_j^{(k)} = 0$ for a measurement yielding the eigenvalue 1 and $S_j^{(k)} = 1$ for the eigenvalue -1 .

The measurements on the input column projects the first column of resource

qubits into the state,

$$|\psi\rangle_{r_{j1}}^{\otimes j} = G^{(1)} M(\vec{S}^{(1)}) |\Psi\rangle_{in}, \quad (2.25)$$

where the operators acting horizontally between rows are given by

$$M(\vec{S}^{(k)}) = M_1(S_1^{(k)}) \otimes M_2(S_2^{(k)}) \otimes \cdots \otimes M_n(S_n^{(k)}), \quad (2.26)$$

with

$$M_j(S_j^{(k)}) = HZ^{S_j^{(k)}}, \quad (2.27)$$

and the vertical operators by

$$G^{(k)} = \prod_{\{(j,k),(j',k)\} \in E} U(\phi_{r_{jk}r_{j'k}}). \quad (2.28)$$

where, again, the set of edges E is represented in Fig. 2.2. Measurements are then performed successively on columns 1 through $l-1$, leaving the output state on the final line of qubits. Immediately, we can see that the evolution from column to column is unitary, and so the entire process can be described by a single unitary operation. In fact, as there is no feed-forward of the measurement outcomes one could in principle make all measurements simultaneously.

In Appendix 2.A we consider more general weighted graph states and more general measurements. However, as the next section will show, the simpler version of the scheme appears to work very well.

2.6 Evaluation of scheme

2.6.1 Unbiased sampling asymptotically

We demonstrate numerically that the scheme gives unbiased sampling (Haar measure) in the asymptotic time limit. More precisely we show that the output state distribution passes a necessary and stringent test, namely that the entanglement probability distribution approaches that associated with the Haar distribution on

pure states.

The entanglement distribution associated with the Haar distribution has received considerable attention recently [25, 26, 27, 28, 31]. The average entropy of entanglement $\mathbb{E}S_A(N_A, N_B)$ of a set of N_A spins was studied already in the 70s and 80s [26, 27] and the explicit solution (“Page’s conjecture”) was conjectured in [28] and proven in [31]:

$$\mathbb{E}S_A(N_A, N_B) = \frac{1}{\ln 2} \sum_{k=2^{N_B+1}}^{2^{N_A+N_B}} \left(\frac{1}{k} - \frac{2^{N_A} - 1}{2^{N_B+1}} \right), \quad (2.29)$$

with the convention that $N_A \leq N_B$ and where $N_A + N_B = N$, the total number of particles.

This can be used to show that the average entanglement is very nearly maximal, meaning close to N_A , for large quantum systems, i.e. $N \gg 1$. Hence one concludes that a randomly chosen state will be nearly maximally entangled with a large probability. Indeed, it was recently shown that the probability that a randomly chosen state will have an entanglement S_A that deviates by more than δ from the mean value $\mathbb{E}S_A(N_A, N_B)$ decreases exponentially with δ^2 [25].

Achieving this entanglement probability distribution is a strong condition to claim one has the true Haar distribution. Often one quantifies multipartite entanglement using “linearised” measures based on purity. For example, a popular measure used for pseudo-random circuits is the Meyer-Wallach entanglement [40], which is related to the average purity of each qubit. However, stabilizer states give exactly the correct purity one would expect from the Haar measure. Nevertheless they do not yield the correct entanglement distribution [41, 42]. The probability distribution of entanglement, $P(S_A)$ associated with stabilizer states sampled uniformly at random is given by Theorem I in [42],

$$P(S_A) = \frac{\prod_{i=1}^{N_A} (2^i + 1)}{\prod_{k=N-N_A+1}^N (2^k + 1)} \cdot \prod_{j=1}^{S_A} \frac{(2^{N-N_A+1-j} - 1)(2^{N_A+j} - 2^{2j-1})}{2^{2j} - 1}, \quad (2.30)$$

where N_A is the number of qubits belonging to Alice and N is the total number

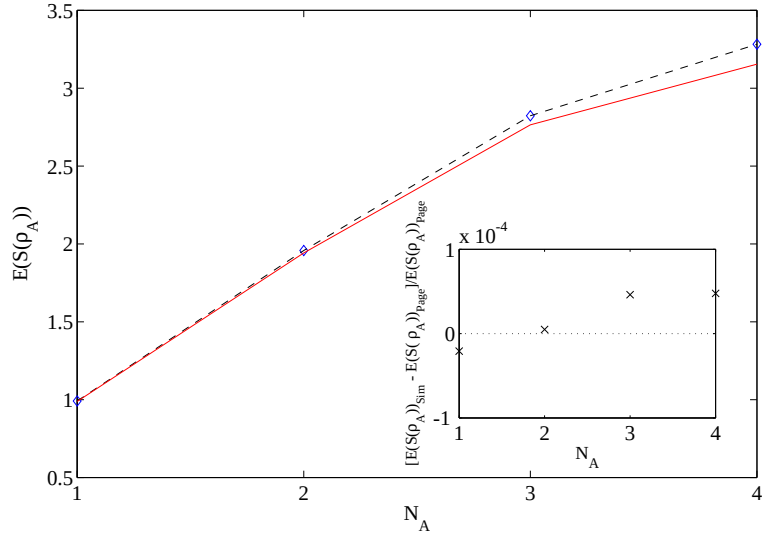


Figure 2.3: The average entanglement, $\mathbb{E}(S(\rho_A))$, (blue diamonds) of our randomized circuits compared with the average expected entanglement given by Page's conjecture (dashed line) for $N = 8$ and various N_A . The solid red line shows the same quantities for stabilizer gates chosen at random. Our final entanglement values are calculated by first specifying an initial input product state of N qubits, where each qubit is chosen at random according to the parametrization $(\alpha|0\rangle + \beta|1\rangle)/\sqrt{\alpha^2 + \beta^2}$. This state is evolved for 10^4 iterations, and averages are then taken over 10^5 separate realisations. In each case the fractional difference is less than 10^{-4} from that expected from true random circuits (see inset).

of qubits. Again $N_A \leq N - N_A = N_B$. The total state is bipartite and pure.

Figures 2.3 and 2.4 show that the output states do indeed follow the correct entanglement statistics, given initially a randomly chosen input product state (see caption of Fig. 2.3). We also add the relevant stabilizer statistics for comparison, which highlight the fact that averaging over stabilizer states is not as good in this regard.

The above considerations strongly indicate that the states coming out of the scheme in the asymptotic time limit are indeed Haar distributed, but they do not constitute an analytical proof.

One could attempt a proof along the lines of [43], by showing that the operators effected by the various measurement outcomes can be strung together to generate any linear combination of elements spanning the Lie Algebra $u(2^N)$. However, we have now restricted ourselves to specific one-parameter families of

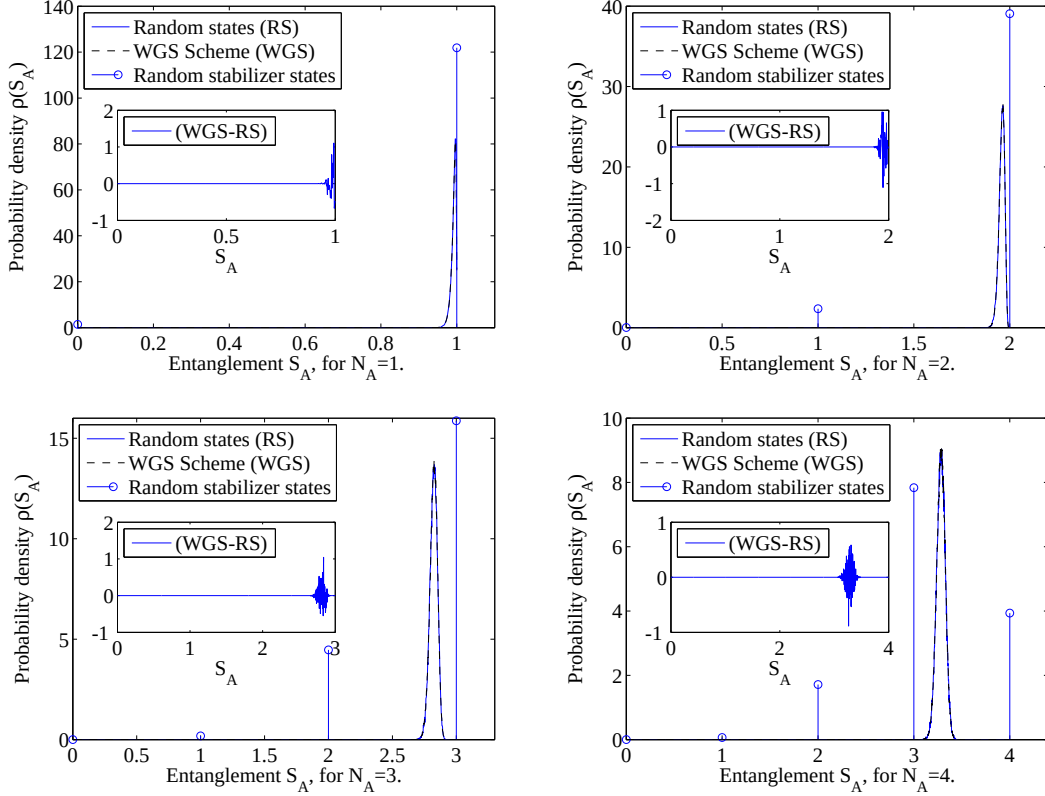


Figure 2.4: Comparisons of the entanglement distributions between the weighted graph states with random initial product states (see caption of Fig. 2.3), and states chosen at random with respect to the Haar measure, for $N = 8$ and $N_A = 1, 2, 3, 4$ (plots from top to bottom). In both cases we calculate 10^5 samples and group into 500 evenly spaced bins. The distributions are then re-scaled such that $\int \rho(S_A) = 1$. Black dashed lines represent the weighted graph state entanglements, and blue solid lines represent the Haar distribution. For comparison, we also include the distributions for stabilizer states chosen at random (solid lines capped with circles), which are given in Eq. (2.30)

unitary operators, and so can no longer invoke the same generic arguments conventionally applied in such approaches. This leads to many difficulties. For example, when trying to demonstrate the appropriate irrationality conditions for the eigenvalues of the evolution operators explicitly, the resulting analytic expressions quickly become intractable. Thus, we have so far been unable to prove that fixed measurements and weighted graph state resources generate a universal set. It should be mentioned, however, that one can immediately see why fixed measurements on graph state resources are not universal. This would correspond to a parameter value of $\phi = \pi$ in our model, for which the eigenvalues of the resulting unitary operators each contain one of the pairs $\pm\pi/3$ or $\pm2\pi/3$. As these operators are periodic, we cannot generate arbitrary linear combinations of their algebra elements, and so we can never cover the full space of unitary operations. For a more in depth analysis along these lines, see Appendix 2.D.

2.6.2 Good sampling in $\text{poly}(N)$ time

In the previous section we considered the sampling in the infinite time limit. In practise one will have a finite time available, and this time should scale as a polynomial function in N , the number of qubits carrying the input state. Under this restriction one cannot generate the Haar measure exactly, however one can hope to obtain a sufficiently good sampling of the state space nevertheless.

To test this for our current scheme, we again use the entanglement of the output states and compare it with the expected entanglement of states chosen at random with respect to the Haar measure. We demand that the difference between the two expected entanglement values is consistently less than some small ε . This will occur after some time t_ε , for a given N and N_A . We then check how t_ε scales with increasing N with fixed N_A , Fig. 2.5.

These results suggest that the time required to achieve the Haar average is linear in the number of qubits and so we expect good scalability of our scheme³.

³Note that the ‘time’ here refers to the number of columns in the weighted graph state that have been measured. Care should therefore be taken in comparing it with the number of two qubit gates necessary in a circuit model randomization. Note that for each time step here,

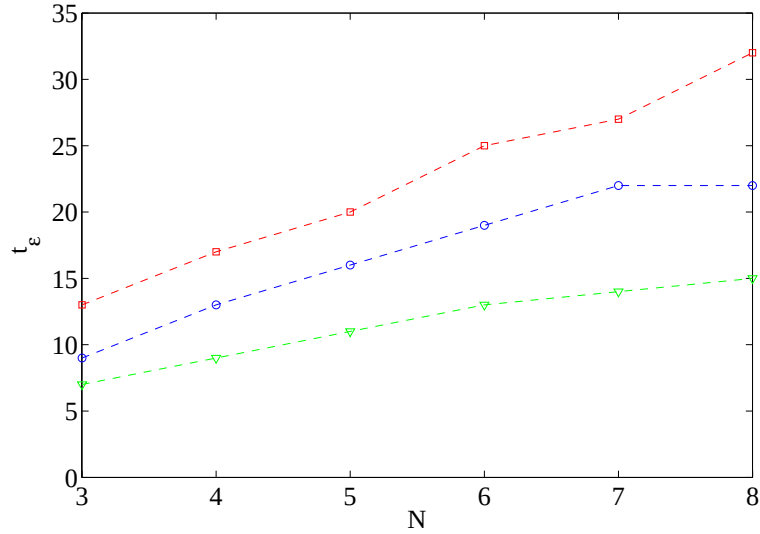


Figure 2.5: (The scaling with N of the time taken for the average entanglement to agree with that associated with the Haar measure to a fixed accuracy $\varepsilon < 0.0001$ (red squares), $\varepsilon < 0.001$ (blue circles) and $\varepsilon < 0.01$ (green triangles). For $N = 2, 3, 4$ averages are over 10^6 realisations. For $N = 5, 6$ averages are over 10^5 realisations and for $N = 7, 8$ averages are over 10^4 realisations. In all cases $\phi = 5\pi/8$ and the initial states are randomly chosen product states (see caption of Fig. 2.3).

It is worth noting here the relevance of the parameter ϕ . Numerical indications suggest this is related to the absolute rate of convergence, with a maximum obtained by a value of approximately $\phi = 5\pi/8$. It can be easily seen that two cases for which our scheme does not work are $\phi = \pi$ and $\phi = 2\pi$. These lead, respectively, to 2D and 1D cluster state resources, for which fixed measurements are not universal. Interestingly, however, we have seen no evidence of any other general restrictions on permissible values of ϕ . An intuitive explanation for this is that the set of possible single time-step evolutions, eq. (2.25), are non-commuting operators. Taken together these may explore the space of unitaries with some complicated dependence on the parameter ϕ .

$2N - 1$ two-qubit gates are needed, which effectively performs $N - 1$ two-qubit gates on the input state, even though only local measurements are made. The experimenter however needs to perform successfully $(2N - 1)l$ two qubit gates in total, where l is the length of the circuit to be implemented.

2.6.3 Realisation

There are several methods and technologies in which states such as the one presented in Fig. 2.2 may be realised. Here we briefly mention two. Firstly, in optical lattices it is possible to implement two-body collisions that implement a Hamiltonian of the form $H = JZ^{(1)} \otimes Z^{(2)}$. To obtain the state in Fig. 2.2 it is then necessary and possible to first implement this Hamiltonian between horizontal neighbours for a time $t = \pi/(4J)$ followed by the implementation of the same pairwise Hamiltonian between vertical pairs for a time $t = \phi/(2J)$ [44]. The ability to generate the desired quantum state in parallel is contrasted by the slight disadvantage that local addressability in such systems is difficult. Recently proposed spin and polariton systems in arrays of optical cavities [46] allows, in principle, for mechanisms analogous to the one described above [47] but where individual nodes of the cluster state reside in distinct cavities and are therefore addressable.

A somewhat different approach to achieve states such as those in Fig. 2.2 is via measurement induced interaction between cavities. The basic idea relies on the insight that one may first entangle the electronic degree of freedom of atoms inside two distinct cavities with the cavity photons. These photons will then leak out of the cavities where they are mixed on a 50/50 beamsplitter and then detected at the two outputs of the beam-splitter. This detection may implement a Bell projection on the atoms enabling the generation of entangled states [48]. Such Bell projections can be used to build large cluster states. These Bell projections may then actually be used directly to implement Controlled NOT gates [49] in a loss tolerant way. Weighted graph states can then be generated via the application of controlled phase gates with rotation angle ϕ . These gates may be obtained from two controlled NOT gates supplemented by local rotations [50].

2.7 Conclusion and outlook

We have proposed a scheme to generate random quantum circuits. In our method, an experimenter prepares a particular type of very entangled state called a weighted graph state. The qubits carrying the input state are then entangled with an edge of the weighted graph state and the experimenter then just performs projective measurements in the $|+\rangle/|-\rangle$ basis. The randomness of the measurement outcomes chooses the particular circuit and no classical random numbers are necessary. We have tested the effectiveness of this scheme in randomising the input state by comparing the entanglement distribution of the output to that associated with the uniform distribution on states. Numerical results strongly suggest these two are identical, and so we may conclude that the scheme is indeed very effective.

From the theoretical perspective several important and interesting questions appear. Firstly one should prove rigorously that the scheme can in fact generate any unitary operation. Along with the random measurement outcomes this would then guarantee that one can generate the Haar measure asymptotically. A possible approach has been detailed in Appendix 2.D, however we quickly find that the problem becomes intractable within this setting. Perhaps another avenue would be to exploit possible mappings between a larger graph state and a weighted graph state. One may then be able to transform the problem to demonstrating universality in a graph state setting (subject to these precise mappings), for which many techniques are already available. Secondly, and in the broader picture, this scheme may also be viewed as an interesting setting to study thermalisation, since there is no classical randomness inserted by hand and yet the evolution appears to maximise the entropy of the input state.

Taking a more practical viewpoint, it seems natural to explore the convergence rates in more detail. The utility of any approach will rely in part on its speed of implementation, and so a comparison against known schemes would seem appropriate.

2.A Generalising the scheme

One could also consider generalising the scheme presented in section 2.5, by including resource qubits in the state $|\psi\rangle_{r_{jk}} = \gamma_{jk}|0\rangle + \delta_{jk}|1\rangle$, along with general two qubit operations between columns. Furthermore, we could also allow measurements in the basis $\{(|0\rangle \pm e^{i\theta_{jk}}|1\rangle)/\sqrt{2}\}$. Defining new operators $\bar{U}_L^{(s)} = \langle 0|_a U_{ab}|0\rangle_a + (-1)^s e^{-i\theta_{jk}} \langle 1|_a U_{ab}|0\rangle_a$ and $\bar{U}_R^{(s)} = \langle 0|_a U_{ab}|1\rangle_a + (-1)^s e^{-i\theta_{jk}} \langle 1|_a U_{ab}|1\rangle_a$, $a = r_{jk}$, $b = r_{jk+1}$ we can write the more general evolution operators as

$$M_j(\vec{S}^{(k)}) = \begin{pmatrix} \gamma\langle 0|_b \bar{U}_L^{S_j^{(k)}} |0\rangle_b + \delta\langle 0|_b \bar{U}_L^{S_j^{(k)}} |1\rangle_b & \gamma\langle 0|_b \bar{U}_R^{S_j^{(k)}} |0\rangle_b + \delta\langle 0|_b \bar{U}_R^{S_j^{(k)}} |1\rangle_b \\ \gamma\langle 1|_b \bar{U}_L^{S_j^{(k)}} |0\rangle_b + \delta\langle 1|_b \bar{U}_L^{S_j^{(k)}} |1\rangle_b & \gamma\langle 1|_b \bar{U}_R^{S_j^{(k)}} |0\rangle_b + \delta\langle 1|_b \bar{U}_R^{S_j^{(k)}} |1\rangle_b \end{pmatrix}.$$

For operators U with entries u_{ij} this can be written as,

$$M_j(\vec{S}^k) = \begin{pmatrix} m_{11} & m_{12} \\ m_{21} & m_{22} \end{pmatrix}. \quad (2.31)$$

where

$$\begin{aligned} m_{11} &= \gamma(u_{11} + (-1)^{S_j^{(k)}} e^{-i\theta_{jk}} u_{31}) \\ &\quad + \delta(u_{12} + (-1)^{S_j^{(k)}} e^{-i\theta_{jk}} u_{32}), \\ m_{12} &= \gamma(u_{13} + (-1)^{S_j^{(k)}} e^{-i\theta_{jk}} u_{33}) \\ &\quad + \delta(u_{14} + (-1)^{S_j^{(k)}} e^{-i\theta_{jk}} u_{34}), \\ m_{21} &= \gamma(u_{21} + (-1)^{S_j^{(k)}} e^{-i\theta_{jk}} u_{41}) \\ &\quad + \delta(u_{22} + (-1)^{S_j^{(k)}} e^{-i\theta_{jk}} u_{42}), \\ m_{22} &= \gamma(u_{23} + (-1)^{S_j^{(k)}} e^{-i\theta_{jk}} u_{43}) \\ &\quad + \delta(u_{24} + (-1)^{S_j^{(k)}} e^{-i\theta_{jk}} u_{44}). \end{aligned}$$

If U is a diagonal unitary operator, then we have the following restriction for unitary evolution,

$$|\gamma|^2 u_{11}^* u_{33} + |\delta|^2 u_{22}^* u_{44} = 0. \quad (2.32)$$

For some applications, such as hiding information about an input state, we are interested in obtaining a randomising operation itself, as opposed to just a state with an expected amount of entanglement. This operation should ideally be unitary, and so the simplest guarantee is to demand that each step in the circuit also corresponds to a unitary operation. We then must impose the above condition from the outset, and so if we wish to adhere to the weighted graph state formalism (2.23), then we are forced to apply only CZ gates between the neighbouring columns of Fig. 2.2.

2.B Measure Theory

For completeness we list here some definitions related to Measure Theory.

2.B.1. DEFINITION. A *measure space* is a triple (Ω, β, μ) where

1. Ω is a set.
2. β is a σ -algebra of subsets of Ω , and
3. μ is a non-negative, countably additive set function on β . That is,

$$(a) \quad \mu : \beta \rightarrow \mathbb{R}_+ \cup \{\infty\}.$$

$$(b) \quad \text{For } B_n \in \beta, n \in \mathbb{N} \text{ and } B_n \cap B_m = \emptyset \text{ if } n \neq m \Rightarrow \mu(\cup_{n \in \mathbb{N}} B_n) = \sum_{n \in \mathbb{N}} \mu(B_n) \text{ and } \mu(\emptyset) = 0.$$

The function μ on a set is known as a *measure*, and assigns to each subset a number representing the size of the subset.

2.B.2. DEFINITION. Let Ω be a set, and 2^Ω its power set (collection of all subsets). Then a subset $\beta \in 2^\Omega$ is called a σ -*algebra* if it satisfies the following properties,

1. β is a non empty set.
2. β is closed under complementation, i.e. $B \in \beta \Rightarrow \Omega \setminus B \in \beta$.

3. β is closed under countable unions, i.e. $B_n \in \beta, n \in \mathbb{N} \Rightarrow \cup_{n \in \mathbb{N}} B_n \in \beta$.

These properties imply that both the empty set $\emptyset$ and Ω itself are in the algebra.

2.C Probability of Correcting a Mistake in the Inverse Problem for Weighted Graphs Resource states

Consider the situation in which we have a set of possible operations, $O = \{O_i\}$. Suppose, we can apply operations from this set any number of times, but only ever at random, and our task is to string them together in some specific order of fixed length. The question of interest is then, for a given sequence, what is the probability of success. Of course, if, after a mistake in one step, we allow ourselves to start again from scratch, then the overall probability of success is simply $P(\text{success}) = \prod_k P_s(k, O)$, where $P_s(k, O)$ is the probability of applying the desired operation at step k . If our set contains N possible operations, and each is applied with equal likelihood, then a string of length m will have a probability of success $P(\text{success}) = 1/N^m$. Thus for finite strings and operation sets, one can eventually expect to carry out the desired task.

Suppose, however, these operations are to be applied to a system or state (perhaps unknown) for which only one copy is available. Now if a mistake is made we cannot start again from scratch, but instead must make a correction before continuing. We introduce an additional set $O^{-1} = \{O_i^{-1}\}$, constructed from the inverse operations of the original set, and demand that these too can only be applied at random. It then follows that mistake at the correction attempt, itself requires a correction (using our original operations O , again drawn at random), and so on until the first error is rectified. The entire correction process for one step leads naturally to a tree like structure were successful branches terminate once the number of successful individual correction attempts is one greater than the number of failures, see Fig. 2.6. The total probability of success for a given

number of allowed attempts is found by adding the probabilities associated to each terminating branch. Clearly, branches can only terminate after an odd number of branch points, and so for the case of $P(O_i) = P(O_i^{-1}) = P(O_j) = P(S)$, the probability of correcting the initial error using at most $2n + 1$ attempts is

$$P_{\text{succ}}(2n+1) = \sum_{j=0}^n S_{\text{new}}(2j+1)P(S)^{j+1}(1-P(S))^j, \quad (2.33)$$

where the function $S_{\text{new}}(j)$ is the number of new branches terminating at stage j .

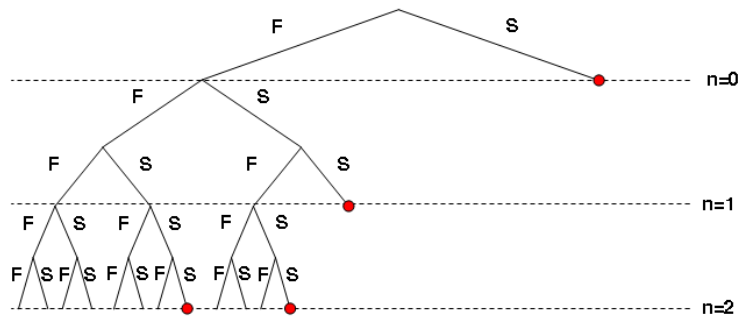


Figure 2.6: The tree structure emerging from successive attempts to correct a mistake, shown for the first $2 \times 2 + 1$ levels. Operations can either succeed (S) or fail (F) to be applied correctly, however the probability of success at each stage is in general dependent on the specific operations realised further up the branch. Overall success is obtained when the number of successful outcomes is one greater than the number that fail. For $n = 2$, we see there are 2 new terminating branches, with the sequences $FSFSS$ and $FFSSS$

2.C.1 Determination of S_{new}

For a branch to terminate exactly at the $2n+1$ th level it must satisfy the following two conditions. 1) The total number of successes in the branch after $2n+1$ applications, $N(S, 2n+1)$, is exactly one greater than the total number of failures, $N(F, 2n+1)$, and 2) The branch has not terminated before the $2n+1$ th level. These imply that $N(S, 2n+1) = n+1$ and that the branch succeeds on the final level i.e. $N(S, 2n) = n$. The strategy is then as follows. We first consider a generic tree of $2n+1$ levels, and calculate the number of branches (or combinations of S 's

and F 's) which satisfy this condition, this is given by $\binom{2n}{n}$. We then subtract from this, the number of branches that have these properties but have arisen from branches that terminated exactly on the $2m + 1$ th level, for all $m < n$. For this, we note that to terminate on the $2m + 1$ th level, we have a sequence already containing $m + 1$ S 's and so if the $2n$ th level is to have the appropriate number of S 's, then we need a further $n - m - 1$ out of $2n - 2m - 1$. This can happen $\binom{2n - 2m - 1}{n - m - 1}$ ways, and so each new branch terminating at level $2m + 1$ contributes this many of times to the number of branches we “thought” could have terminated at level $2n + 1$. Thus, for our final level we have the following recurrence relation

$$S_{\text{new}}(2n + 1) = \binom{2n}{n} - \sum_{m=0}^n S_{\text{new}}(2m + 1) \binom{2n - 2m - 1}{n - m - 1}, \quad (2.34)$$

for which we find the solution in terms of the Catalan numbers,

$$S(2n + 1) = C_n = \frac{1}{n + 1} \binom{2n}{n}. \quad (2.35)$$

2.D Analytic considerations: Universality via Lie Algebras

For a given collection of operators in a Lie group $\mathcal{G}$, we begin by calculating the corresponding elements of the Lie algebra g . In our model, we are considering the 2^N operators $U_s = GM(\vec{s})$, corresponding to the evolutions $|\psi\rangle_f = U_s|\psi\rangle_i$. As we are interested only in schemes resulting in unitary evolutions, each operator U_s has a corresponding element (Hamiltonian) H_s of the Lie Algebra $u(2^N)$ given by $U = \exp(iH)$. Our first task is to find these elements, and demonstrate that all but one of the eigenvalues of each are irrational in multiples of π . Successive application of these U operators then allow the construction of any operator of

the form $U^n(\vec{s}) = e^{inH_s}$, to arbitrary accuracy. Furthermore, we can construct any operation generated by a linear combination $\alpha H_1 + \beta H_2$ of any two such elements H_1 and H_2 via

$$e^{i(\alpha H_1 + \beta H_2)} = \lim_{n \rightarrow \infty} (e^{i\frac{\alpha}{n}H_1} e^{i\frac{\beta}{n}H_2})^n. \quad (2.36)$$

We can also generate a third element, H_3 , given any two algebra elements, H_1 and H_2 by virtue of the Lie Bracket, $H_3 = i[H_1, H_2]$. These are realised via the applications

$$e^{[H_1, H_2]} = \lim_{n \rightarrow \infty} (e^{-iH_1/\sqrt{n}} e^{iH_2/\sqrt{n}} e^{iH_1/\sqrt{n}} e^{-iH_2/\sqrt{n}})^n. \quad (2.37)$$

Thus we can build up a potentially large set of elements, provided the commutators do not quickly vanish. If, within such a set, there exists a collection of $(2^N)^2$ linearly independent generators, each having the irrational eigenvalue property above then by (2.36) we can construct any element of the Lie Algebra, and thereby generate any element of the Lie Group. In this sense the initial operations U_s are universal. Note, this basis need not contain all of the 2^{2N} original operators, as we shall see later.

The three key steps for completing a proof in this framework are summarised as follows,

1. Find the Hamiltonians corresponding to each operator U_s
2. Generate a spanning set of linearly independent generators from the initial elements H_s , using the Lie Bracket and nested Lie Brackets. For our case, we need to construct (2^{2N}) such elements.
3. Check that all but (at most) one of the eigenvalues of each generator in the basis set is an irrational multiple of π and that each of these eigenvalues is not a rational multiple of any other of the same generator.

One could hope that by proving this for the case of two qubits ($N = 2$), you could readily extend for all N . However it is not obvious that this follows

immediately. For example, one does not have the option of generating any two qubit unitary, through this method, and then applying it arbitrarily to any pair of qubits in a larger system. Nevertheless, it does seem likely that this extension should be possible, and so we begin by considering this simpler case. The first task is then to find the Hamiltonians for each of the four operators $U_s = GM(\vec{s})$. For our setup we have

$$G = \prod_{j>i} G_{ij} = G_{12} = \text{diag}(1, 1, 1, e^{-i\phi}). \quad (2.38)$$

and $M(\vec{s})$ given by the tensor product $M(\vec{s}) = M(s_1) \otimes M(s_2)$ of the elementary evolutions

$$M(s_1) = HZ^{s_1}. \quad (2.39)$$

Explicitly, these unitary operators are represented by the matrices

$$\begin{aligned} U_1 &= \frac{1}{2} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ e^{-i\phi} & -e^{-i\phi} & -e^{-i\phi} & e^{-i\phi} \end{pmatrix}, U_2 = \frac{1}{2} \begin{pmatrix} 1 & -1 & 1 & -1 \\ 1 & 1 & 1 & 1 \\ 1 & -1 & -1 & 1 \\ e^{-i\phi} & e^{-i\phi} & -e^{-i\phi} & -e^{-i\phi} \end{pmatrix}, \\ U_3 &= \frac{1}{2} \begin{pmatrix} 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & 1 \\ e^{-i\phi} & -e^{-i\phi} & e^{-i\phi} & -e^{-i\phi} \end{pmatrix}, U_4 = \frac{1}{2} \begin{pmatrix} 1 & -1 & -1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ e^{-i\phi} & e^{-i\phi} & e^{-i\phi} & e^{-i\phi} \end{pmatrix}. \end{aligned} \quad (2.40)$$

Numerically, calculating the Hamiltonians is straight forward, for a given parameter ϕ , by taking the logarithms $H_{s,\phi} = -i \log(U_{s,\phi})$. We can then construct a set of generators and test for linear independence. This was done by forming a 16×16 matrix with each column corresponding to the concatenation of the columns in one of the 16 individual generators. Linear independence then corresponds to a non vanishing determinant. A simple recursive scheme for generating promising

matrices is the following.

$$H_j = i[H_2, H_{j-1}] \quad j = 5 \dots 16, \quad (2.41)$$

where $H_{1\dots 4}$ is constructed from the operators $U_{1\dots 4}$. This scheme was used for the explicit numerical calculation of the absolute values of the determinant over a range of ϕ in the interval $[0, 2\pi]$. Fig. 2.7 shows that within resolutions of $2\pi/10000$, the determinant is non-zero over the range $0 \leq \phi \leq 2\pi$, getting very close to zero in the vicinity of $\phi = 0$ and $\phi = 2\pi$. This suggests that the above scheme does indeed generate a basis of generators over nearly the entire range of ϕ . In fact, there appears to be many such schemes which would generate a suitable basis (a second is shown in Fig. 2.7). It is interesting to note that even if the additional zeros suggested by the plots are exact, these can be removed by picking a different construction for those values. However, in all sets studied, the determinant tends to zero close to $\phi = 2\pi$. It is at these parameter values that the evolution to the Haar average appears to converge most slowly.

The second point to notice is that the determinant does not necessarily vanish for $\phi = \pi$, despite the fact that it is known these sets of gates are not universal. The reason for this is likely that the eigenvalues of $U_{s,\pi}$ are no longer irrational in π (they each contain either the pairs $\pm\pi/3$ or $\pm 2\pi/3$), and so the generators are not realisable in the manner of (2.37). One would expect that there may be other values of ϕ for which 16 linearly independent generators with eigenvalues irrational in π cannot be found. For example, there will be an eigenvalue of $\pi/2$ and π in H_1 for $\phi = \arctan(4/3) - \pi$, however in this case we still see convergence to the Haar average (Fig. 2.8) suggesting that a 16 element basis can be found without making use of this element. In fact, it seems that the operations U_2 and U_3 are universal in themselves, which may be easier to prove as they share the same eigenvalues.

2.D.1 Problems

This discussion, though suggestive, has nevertheless revolved around numerical results only. Unfortunately, attempts to extend this analytically have run into considerable problems. These originate in step 1, when we try calculate the required Hamiltonians. A brute force approach, by taking the matrix logarithms, would require solving a fourth order polynomial equation. Even in MAPLE, a straightforward attempt has run into difficulties. While H_1 has been found, it is very cumbersome, furthermore 50 hours of CPU time failed to produce the next term H_2 , even when simplified to $\phi = \pi/2$, with indications that the further terms will have similar problems. Should any expressions finally be found, perhaps via more intelligent calculations methods, we should still expect these to be of at least the complexity of H_1 .

The second issue is proving that the eigenvalues of the generators are irrational. For the simple case of $U_{1,\pi/2}$ MAPLE will calculate the four eigenvalues as

$$\lambda_1^{1,\pi/2} = \pi, \quad (2.42)$$

$$\lambda_2^{1,\pi/2} = \arctan\left(\frac{4}{3} + \frac{\sqrt{7}}{3}\right), \quad (2.43)$$

$$\lambda_3^{1,\pi/2} = -\frac{1}{2}\pi - \arctan\left(\frac{4}{3} + \frac{\sqrt{7}}{3}\right), \quad (2.44)$$

$$\lambda_4^{1,\pi/2} = 0. \quad (2.45)$$

While as an example the eigenvalue $\lambda_2^{2,\pi/2}$ is given by

$$\begin{aligned} \lambda_2^{2,\pi/2} &= i \log\left(\frac{1}{6}C + \frac{1 + \frac{2}{3}i}{C} + \frac{1}{6} + \frac{1}{6}i\right); \\ C &= (6\sqrt{237} - 92 - 2i)^{1/3}. \end{aligned} \quad (2.46)$$

There will be 64 such expressions in general, (though some are constants or zero and at least 4 pairs are identical), all of which must be shown to be irrational (at least at some parameter value).

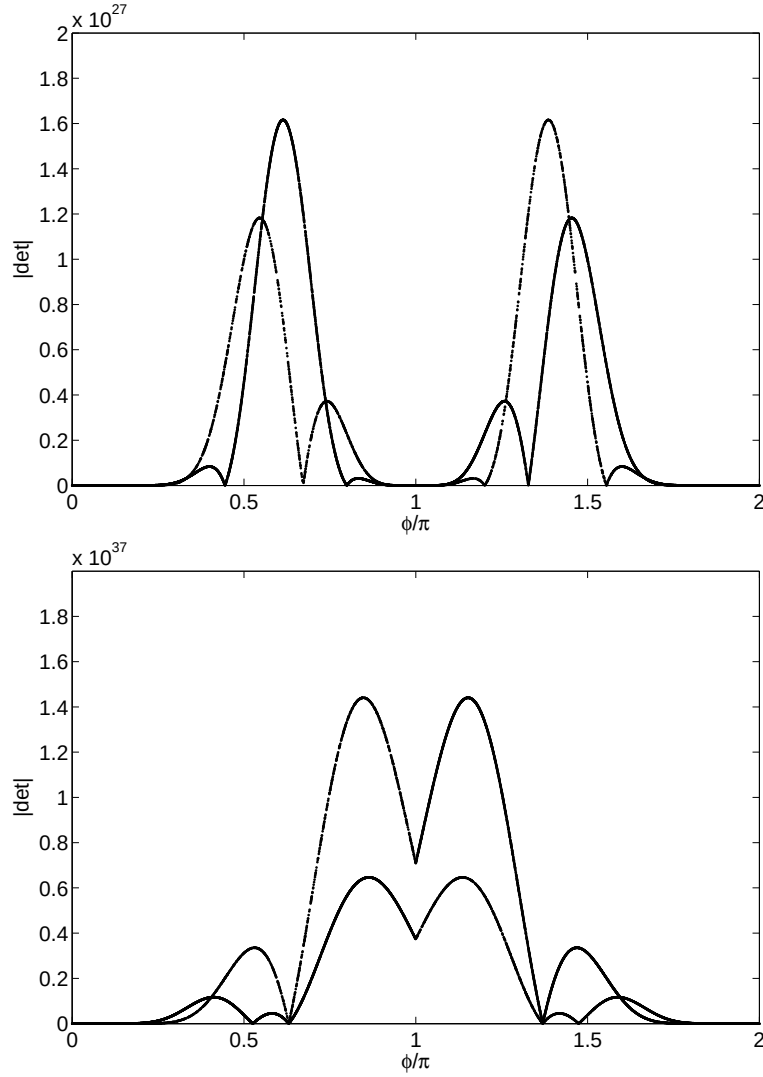


Figure 2.7: Tests of linear independence for a range of ϕ from 0 to 2π at increments of $2\pi/10000$. We calculate the absolute value of the determinant formed from 16 generators given by two schemes. The plot on the top is for the construction (2.41), $H_{1\dots 4}$; $H_j = i[H_2, H_{j-1}]$, $j = 5 \dots 16$. The plot on the bottom uses $H_{1\dots 4}$; $H_j = i[H_2, H_{j-1}]$, $j = 5 \dots 10$; $H_j = i[H_3, H_{j-1}]$, $j = 11 \dots 16$. In both cases $|det| \neq 0$ at $\phi = \pi$, though this is more pronounced for the bottom graph.

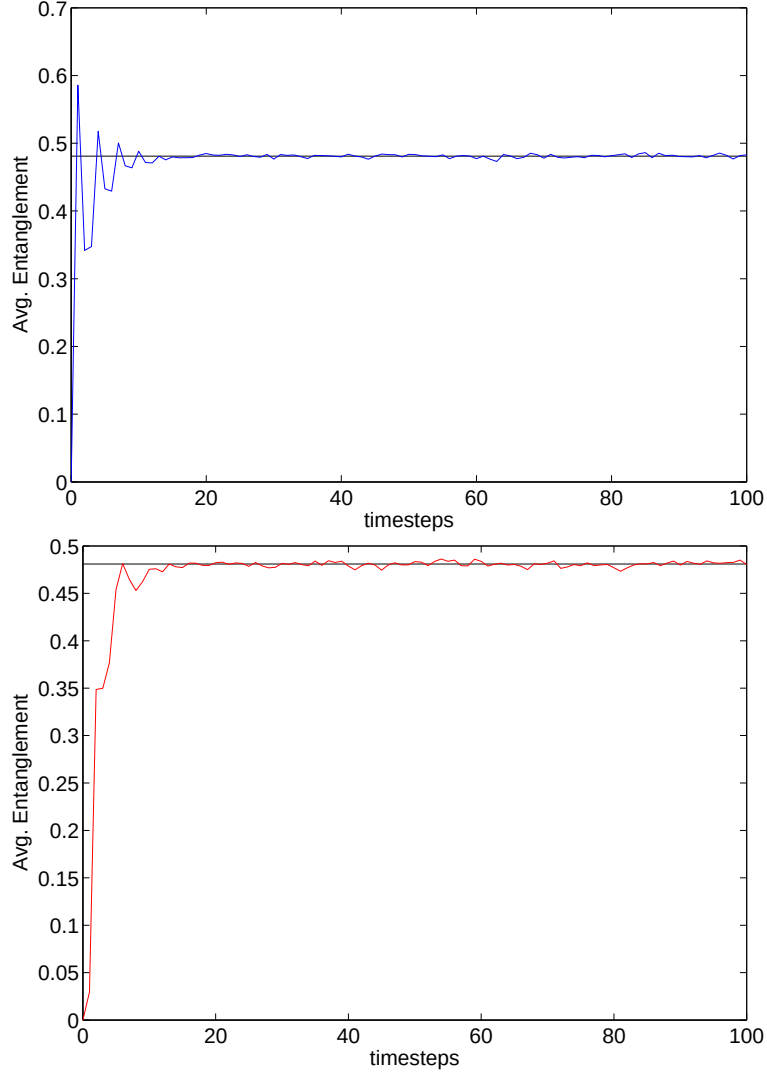


Figure 2.8: Plots of average entanglement against time for $\phi = \arctan(4/3) - \pi$. The Hamiltonian H_1 has more than one eigenvalue irrational in π , however, we still obtain convergence to the Haar average suggesting that it need not be included as an element in a linearly independent basis. The bottom plot shows that when U_1 and U_4 are ignored, we still obtain the desired average ($\phi = \pi/2$). Solid black lines are the expected Haar average. Averaged over 10000 realisations.

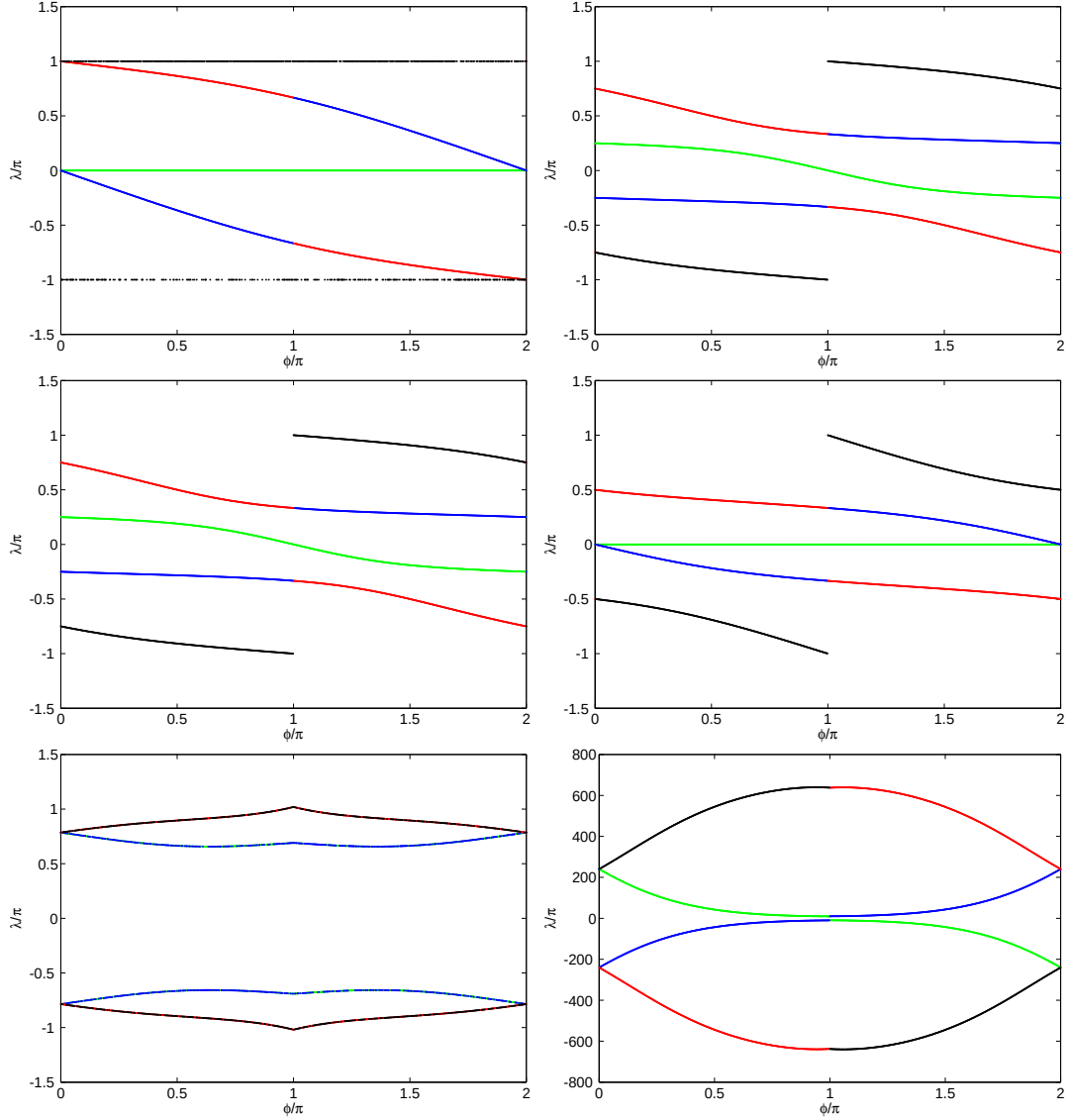


Figure 2.9: Eigenvalues of selected H_j for the construction (2.41). From left to right, top to bottom, H_1 , H_2 , H_3 , H_4 , H_5 and H_{10} . Numerically the eigenvalues were ordered in size for each ϕ , in order of increasing eigenvalues we have the green, blue, red and black points respectively. This does not correspond to the actual behaviour of a given eigenvalue when considered from the analytic expressions (where available). The eigenvalues of H_2 and H_3 can be shown to be identical.

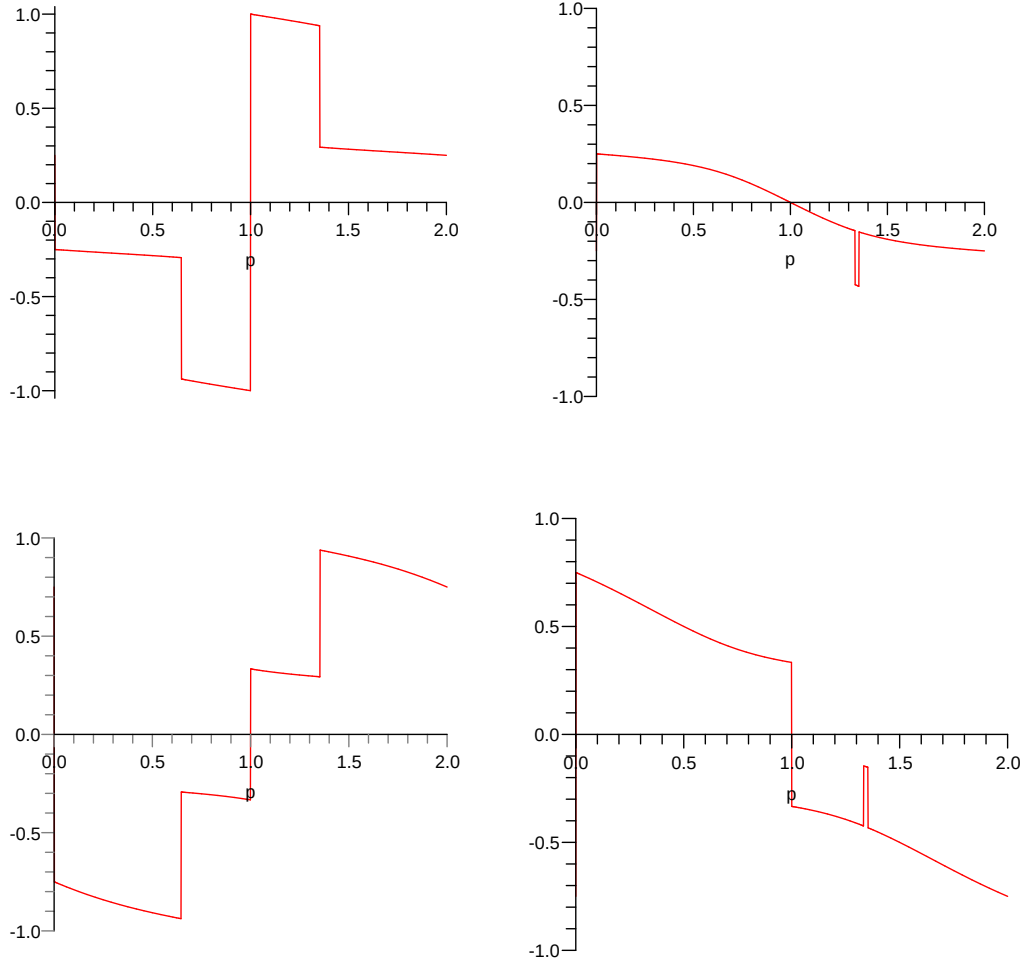


Figure 2.10: Eigenvalues (scaled by π) against $p = \phi/\pi$ of H_2 plotted from exact expressions in MAPLE. These do not correspond to the eigenvalue colourings used in Fig.2.9, but nevertheless give the same distribution when combined (ignoring vertical ‘discontinuities’).

Part II

Continuous Variables and Master Equations

3.1 Introduction

One of the key ingredients for the remainder of this thesis is the class of so called Gaussian states. These play an important role in quantum information, in part due to their compact mathematical description, but also because they are the most experimentally accessible states using current technology. In what follows we will provide a brief introduction to the techniques used to describe and work with them. For a more in depth exposition, we refer the reader to any of the following references [60, 57] or the book by Holevo [56]. For some background motivation in regards to various phase space functions, see [58].

3.2 Phase Space Methods and Gaussian states

Our primary point of interest is the phase space describing a system of N degrees of freedom. This is taken as the symplectic manifold (Ξ, σ) , where Ξ is a real $2N$ -dimensional vector space possessing a symplectic form $\sigma : \Xi \times \Xi \rightarrow \mathbb{R}$. Symplectic forms, over a vector space, are nondegenerate bilinear antisymmetric forms and

so can be conveniently expressed as a matrix

$$\sigma(\eta, \nu) = \eta^T \sigma \nu, \quad (3.1)$$

where, for a fixed choice of basis $\{\mathbf{e}_k\}$, $\sigma_{k,l} = \sigma(\mathbf{e}_k, \mathbf{e}_l)$. The remaining conditions require this matrix to be skew-symmetric and non-singular (and thus even dimensional). In fact, it turns out every finite symplectic vector space is locally diffeomorphic to a space with the following basis¹, $(e_1, e_2, \dots, e_N, \dots, e'_1, e'_2, \dots, e'_N)$, where

$$\begin{aligned} \sigma(e_k, e_l) &= \sigma(e'_k, e'_l) = 0, \\ \sigma(e_k, e'_l) &= \delta_{kl}. \end{aligned} \quad (3.2)$$

In this basis, the symplectic form can easily be written as the following matrix,

$$\sigma = \begin{bmatrix} 0 & \mathbb{I}_n \\ -\mathbb{I}_n & 0 \end{bmatrix}. \quad (3.3)$$

We can make the connection to Quantum Mechanics via the canonical operators R_k . For any system of n canonical degrees of freedom, such as n harmonic oscillators, or n modes of a field, we can combine the $2n$ conjugate operators corresponding to position and momentum into a convenient row vector,

$$R = (X_1, X_2, \dots, X_n, P_1, P_2, \dots, P_n)^T. \quad (3.4)$$

We then impose the usual canonical commutation relations (CCR), which take the form

$$[R_k, R_l] = i\sigma_{kl}, \quad (3.5)$$

One may also choose a mode-wise ordering of the operators,

$$R^{\text{m-w}} = (X_1, P_1, \dots, X_n, P_n)^T,$$

¹This is a consequence of a theorem by Darboux.

and in which case the symplectic matrix takes on the form,

$$\sigma^{\text{m-w}} = \bigoplus_{j=1}^n \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}. \quad (3.6)$$

These two orderings are easily interchanged under the operation of a $2n \times 2n$ permutation matrix, P , which transforms between the vectors as $R = PR^{\text{m-w}}$, and is given explicitly as,

$$P_{jk} = \begin{cases} \delta_{j,2k-1} & j \leq n \\ \delta_{n+j,2k} & k \leq n \end{cases}, \quad (3.7)$$

Similarly, we have

$$\sigma = P\sigma^{\text{m-w}}P^T. \quad (3.8)$$

Canonical transformations of the vectors $S : \vec{R} \rightarrow \vec{R}'$ are then the real $2n$ -dimensional matrices S which preserve the kinematic relations specified by the CCR. That is, the elements transform as $R'_a = S_{ab}R_b$, under the restriction,

$$S\sigma S^T = \sigma. \quad (3.9)$$

This condition defines the real $2n$ -dimensional symplectic group $Sp(2n, \mathfrak{R})$, and so we can say the phase space adopts the structure of a symplectic vector space. For any element $S \in Sp(2n, \mathfrak{R})$, the transformations $-S$, S^T and S^{-1} are also symplectic matrices, and the inverse can be found from $S^{-1} = \sigma S^T \sigma^{-1}$.

3.2.1 Phase space representations

Rather than considering unitary operators acting on states in a Hilbert space, we can instead think of all the quantum dynamics taking place on phase space. States, and operators, are then represented by c -number phase space functions. Common approaches assign to each density matrix ρ a weight function $w(\alpha)$ taking a complex argument α which represents a point (p, q) in phase space. To

each operator $\hat{O}$ we represent a function $f(\alpha)$, expectation values $\langle \hat{O} \rangle$ are then written as integrals over the complex plane,

$$\text{tr}(\rho \hat{O}) = \int w(\alpha) f(\alpha) d^2\alpha. \quad (3.10)$$

The differential $d^2\alpha = d(\text{Re}\alpha)d(\text{Im}\alpha)$ is a real element proportional to the phase space element $dpdq$ and so the integral is over all possible states of the system. While one may be tempted to regard the weight function $w(\alpha)$ as a probability function, in general this is not true. It is clear from the commutation relations above that the choices of the functions $f(\alpha)$ (and $w(\alpha)$) are not unique. For example, a simple function such as $|\alpha|^2$ could be equivalently written as $\alpha^*\alpha$, $\alpha\alpha^*$. However, the same can not be said of non-commuting operators such as $a^\dagger$ and a , for which such expressions are not equivalent. Any starting point therefore relies on first adopting a particular ordering convention. Common choices are normal and antinormal ordering, where all creation operators a are written on the left, respectively right, of the annihilation operators in any operator product. An example of the first type can be found in the P -Representation, where operators are expanded as a power series of normally ordered products (it is interesting to note however, that the weight function assumes the reverse ordering of the density operator). The second type is the basis for the correspondence in the Q -function. While a third convention, the symmetrically ordered product $\{a^m(a^\dagger)^n\}_{sym}$, which is the average of all ways of ordering the operators, can be identified with the Wigner function.

These associations implicitly require an appropriate corresponding basis, in which the functions describing the states can be evaluated. Such basis must necessarily form a complete, though not always orthonormal set, the prime example of which being that of the coherent states [59].

3.2.2 The quantum characteristic function

For our purposes, we shall instead opt to use the characteristic function $\chi_\rho(\xi)$, which we define by first introducing the Weyl operator

$$W_\xi = \mathbf{e}^{i\xi^T \sigma \vec{R}}, \quad \xi \in \mathcal{R}^{2n}. \quad (3.11)$$

Then the quantum characteristic function is given by

$$\chi_\rho(\xi) = \text{tr}[\rho W_\xi]. \quad (3.12)$$

Each function uniquely determines a quantum state, and the two are related through a Fourier-Weyl transform,

$$\rho = \frac{1}{(2\pi)^{2n}} \int d^{2n}\xi \chi_\rho(-\xi) W_\xi. \quad (3.13)$$

We then define the set of Gaussian states as those with Gaussian characteristic functions. It should be noted, that we could have instead based our definition on one of the alternative phase space functions. The corresponding characteristic functions would then be taken over the normally, or anti-normally ordered Weyl operator, and so if any one characteristic function is Gaussian then so will the others. Similarly, as the Wigner, P and Q functions are found from the respective Fourier transforms, Gaussian states defined according to any of these phase space functions will be equivalent [58]. It then suffices to concern ourselves with states which have (Wigner) characteristic functions of the form

$$\chi_\rho(\xi) = \chi_\rho(0) \mathbf{e}^{-\frac{1}{4}\xi^T \Gamma \xi + D^T \xi}, \quad (3.14)$$

where Γ is a $2n \times 2n$ real matrix and $D \in \mathcal{R}^{2n}$ is a vector. Thus, a Gaussian characteristic function, and therefore any Gaussian state, can be completely specified by $2n^2 + n$ real parameters. The first moments give the expectation values of the canonical coordinates $d_j = \text{tr}[R_j \rho]$ and are related to D by $d = \sigma^{-1} D$, while the

second moments make up the covariance matrix $\mathcal{C}$, defined by²

$$\mathcal{C}_{j,k} = 2\mathbf{Re} \, \mathbf{tr}[\rho(R_j - \langle R_j \rangle_\rho)(R_k - \langle R_k \rangle_\rho)]. \quad (3.15)$$

These are related to Γ by the relation $\Gamma = \sigma^T \mathcal{C} \sigma$. It is often the case that only the entanglement properties of a given state are of interest. As the vector d can be made zero by local translations in phase space, one can specify the state entirely using the simpler relation,

$$\mathcal{C}_{j,k} = 2\mathbf{Re} \, \mathbf{tr}[\rho R_j R_k]. \quad (3.16)$$

However, in this work we shall predominantly use the relation (3.15). Using this convention, we mention two states of particular interest. First, the vacuum state can be expressed succinctly as $\mathcal{C} = \mathbb{I}_{2n}$. The second state, which we will make use of frequently, is the n -mode thermal state and takes on a simple diagonal form,

$$\mathcal{C}_{j,k} = \delta_{jk} \left(1 + \frac{2}{e^{\omega_j/T} - 1} \right). \quad (3.17)$$

where ω_j is the frequency of the j^{th} mode, and the equilibrium temperature is given by T .

3.3 Operations on Gaussian States

We now consider Gaussian transformations. As the $\hat{R}_j$ are Hermitian and irreducible, given any real symplectic transform S , the Stone Von Neumann theorem tells us there exists a unique unitary transformation U_S acting on $\mathcal{H}$ such that $U_S W_\xi U_S^\dagger = W_{S\xi}$. Of particular interest are those operators, U_G , which transform Gaussian states to Gaussian states. To this end, we consider the infinitesimal generators G , of Gaussian unitaries $U_G = e^{-i\epsilon G} = \mathbb{I} - i\epsilon G + o(\epsilon^2)$. Then to preserve the (Weyl) canonical commutation relations, the generators G must have the form

²This can be related to the mode-wise ordered covariance matrix using the relation $\mathcal{C} = P\mathcal{C}^{\text{m-w}}P^T$.

$G = \sum_{j,k=1}^{2n} g_{jk}(R_j R_k - R_k R_j)/2$ [57]. It follows that Hamiltonians quadratic in the canonical position and momentum operators (and correspondingly, the creation and annihilation operators) will be Gaussian preserving and in particular, the Hamiltonian for n simple harmonic oscillator, $H = \sum_{j=1}^n \omega_j a_j^\dagger a_j$. It is for this reason that harmonic oscillators provide such a useful testing ground for many body systems.

An additional, though simple, property worth highlighting is the action of the partial trace. Using the expression for the density matrix (3.13), it is straightforward to see the effect of the partial trace operation on the characteristic function. If we take a mode-wise ordering of the vector $\vec{R} = (\vec{R}_1, \vec{R}_2)$, where $\vec{R}_1$ and $\vec{R}_2$ split two subspaces of n_1 and n_2 conjugate variables corresponding to partitions of the state space of ρ into $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$, then the partial trace over $\mathcal{H}_2$ is given by

$$\text{tr}_2[\rho] = \frac{1}{(2\pi)^{2n_1}} \int d^{2n_1} \xi_1 \chi_\rho(-\xi_1) W_{\xi_1}. \quad (3.18)$$

That is, we need only consider the characteristic function $\chi(\xi_1)$ associated to the vector $\vec{R}_1$. At the level of covariance matrices, we simply discard elements corresponding to variances including any operators in $\vec{R}_2$, and so the partial trace of a Gaussian state will itself remain Gaussian.

3.3.1 Time-independent evolution

From the above a general, Gaussian preserving time-independent Hamiltonian will be of the form,

$$H = \frac{1}{2} R^T K R, \quad (3.19)$$

where $K = K^\dagger$ guarantees Hermiticity. We can show in a fairly straightforward manner how the covariance matrix evolves under this action. Most easily, this can be seen by starting from the Heisenberg equation,

$$\dot{R}_j(t) = i[H, R_j]. \quad (3.20)$$

Inserting the linear Hamiltonian above, and recalling the commutation relations (3.5), we have

$$\begin{aligned}
2\dot{R}_j(t) &= i \sum_{r,s}^{2n} R_r K_{rs} R_s R_j - R_j R_r K_{rs} R_s \\
&= i \sum_{r,s}^{2n} K_{rs} (R_r [R_s, R_j] - [R_j, R_r] R_s) \\
&= i \sum_{r,s}^{2n} K_{rs} (R_r i\sigma_{sj} - i\sigma_{jr} R_s) \\
&= - \sum_{r,s}^{2n} \sigma_{js}^T K_{rs} R_r + \sum_{r,s}^{2n} \sigma_{jr} K_{rs} R_s.
\end{aligned} \tag{3.21}$$

Now recalling $K = K^T$ and $\sigma^T = -\sigma$ we have

$$\dot{R}(t) = \sigma K R, \tag{3.22}$$

with the solution,

$$R(t) = e^{\sigma K t} R(0) = \mathcal{M} R(0). \tag{3.23}$$

If such a system starts out in a Gaussian state, it will remain Gaussian throughout its entire evolution. This means we need only concern ourselves with the covariance matrix $\mathcal{C}(t)$, which is readily computed by finding the time evolution of the expectation values of pairs on conjugate operators,

$$\langle R_j(t) R_k(t) \rangle = \sum_{l,m}^{2n} \mathcal{M}_{jl} \mathcal{M}_{km} \langle R_l(0) R_m(0) \rangle, \tag{3.24}$$

and similarly for products of expectation values. It then follows that

$$\mathcal{C}_{jk}(t) = \sum_{l,m}^{2n} \mathcal{M}_{jl} \mathcal{M}_{km} \mathcal{C}_{lm}(0), \tag{3.25}$$

or in matrix form,

$$\begin{aligned}\mathcal{C}(t) &= \mathcal{M}\mathcal{C}(0)\mathcal{M}^T \\ &= e^{\sigma K t}\mathcal{C}(0)e^{-K^T\sigma t}.\end{aligned}\tag{3.26}$$

Again, K is a $2n \times 2n$ matrix and so we can immediately see the convenience of dealing with a system in this form. In fact, we are often interested in Hamiltonians which are only quadratic in position and momentum, $H = \frac{1}{2} \sum_{j,k=1}^n X_j V_{jk} X_k + P_j T_{jk} P_k$. In this case, making the choice (3.4) for R allows for a little computational simplification, as then the matrix K takes on the block diagonal form $K = \begin{pmatrix} V & 0 \\ 0 & T \end{pmatrix}$. This gives us immediately [65],

$$\begin{bmatrix} \mathcal{C}_{XX}(t) & \mathcal{C}_{XP}(t) \\ \mathcal{C}_{PX}(t) & \mathcal{C}_{PP}(t) \end{bmatrix} = \exp\left(\begin{bmatrix} 0 & T \\ -V & 0 \end{bmatrix} t\right) \begin{bmatrix} \mathcal{C}_{XX} & \mathcal{C}_{XP} \\ \mathcal{C}_{PX} & \mathcal{C}_{PP} \end{bmatrix} \exp\left(\begin{bmatrix} 0 & -V \\ T & 0 \end{bmatrix} t\right),\tag{3.27}$$

where the omitted time dependence implies the initial state. The ground state of such a Hamiltonian is given by $\mathcal{C} = \sqrt{TV^{-1}} \oplus \sqrt{VT^{-1}}$ [65]. On the other hand, we may often want to work with a Hamiltonian defined in terms of the creation and annihilation operators,

$$a_j^\dagger = \frac{1}{\sqrt{2}}(X_j - iP_j), \quad a_j = \frac{1}{\sqrt{2}}(X_j + iP_j).\tag{3.28}$$

For convenience these may be collected in a vector $A^{(c)}$, where we have introduced the notation of a bracketed superscript c to distinguish when vectors or matrices are defined in relation to these operators. The ordering can be chosen in such a way that they obey the commutation relations,

$$[A_j^{(c)}, A_k^{(c)}] = \sigma_{jk},\tag{3.29}$$

provided that the transformation from the conjugate operators, $A^{(c)} = \Omega R$, satisfies the following condition, $i\Omega\sigma\Omega^T = \sigma$. Relating these back to the choice of R

in (3.4), the vector of mode operators can be written in the form $A^{(c)} = (A, A^\dagger)^T$,

$$A^{(c)} = (a_1, a_2, \dots, a_n, a_1^\dagger, a_2^\dagger, \dots, a_n^\dagger)^T = \Omega R, \quad (3.30)$$

where the transformation Ω is given explicitly by the matrix,

$$\Omega = \frac{1}{\sqrt{2}} \begin{pmatrix} \mathbb{I}_n & i\mathbb{I}_n \\ \mathbb{I}_n & -i\mathbb{I}_n \end{pmatrix}, \quad \Omega^{-1} = \Omega^\dagger = \frac{1}{\sqrt{2}} \begin{pmatrix} \mathbb{I}_n & \mathbb{I}_n \\ -i\mathbb{I}_n & i\mathbb{I}_n \end{pmatrix}. \quad (3.31)$$

In terms of these operators, a general linear Hamiltonian takes on the form

$$H = \frac{1}{2} A^{(c)T} K^{(c)} A^{(c)} = \frac{1}{2} R^T [\Omega^T K^{(c)} \Omega] R, \quad (3.32)$$

The dynamics of which can be solved using the Heisenberg equation along the lines of (3.21) giving the differential equation,

$$\dot{A}^{(c)}(t) = -i\sigma K^{(c)} A^{(c)}. \quad (3.33)$$

Of course, as we will mostly be interested the evolution of the covariance matrix all we really need to do is substitute $K = \Omega^T K^{(c)} \Omega$ into our solution (3.26).

3.3.2 The Rotating Wave Approximation

A simpler dynamics can be obtained if we first make the rotating wave approximation. This kind of approximation is common in Quantum Optics, where one is typically describing atomic systems in a radiation field. As we shall see below, it amounts to neglecting non energy-conserving terms such as $a_j^\dagger a_k^\dagger$ and $a_j a_k$, that is terms which correspond to the simultaneous excitation (or de-excitation) of a pair of oscillators.

Let us consider a system of two oscillators coupled by a spring. For simplicity, we assume their respective ground state energies are zero, and so the Hamiltonian

can be written as,

$$H = \Omega a^\dagger a + \omega b^\dagger b + (\lambda a + \lambda^* a^\dagger)(b + b^\dagger). \quad (3.34)$$

If we now transform to the interaction picture $\tilde{H} = e^{iH_0 t} H e^{-iH_0 t}$, that is a frame rotating with the uncoupled system $H_0 = \Omega a^\dagger a + \omega b^\dagger b$ we find,

$$\begin{aligned} \tilde{H} &= e^{iH_0 t} (H_0 + H_I) e^{-iH_0 t} \\ &= H_0 + e^{i(\Omega a^\dagger a + \omega b^\dagger b)t} H_I e^{-i(\Omega a^\dagger a + \omega b^\dagger b)t} \\ &= \Omega a^\dagger a + \omega b^\dagger b + \lambda e^{-i(\Omega + \omega)t} a b + \lambda^* e^{i(\Omega - \omega)t} a^\dagger b \\ &\quad + \lambda e^{-i(\Omega - \omega)t} a b^\dagger + \lambda^* e^{i(\Omega + \omega)t} a^\dagger b^\dagger, \end{aligned}$$

where

$$H_I = (\lambda a + \lambda^* a^\dagger)(b + b^\dagger).$$

In the quantum optical setting we are often interested in situations when an incident electromagnetic field is close to resonance with an atomic transition. The analogous case with our oscillator model is that $\Omega \approx \omega$ and so terms like $e^{i(\Omega + \omega)t}$ will oscillate very rapidly. Over appreciable timescales their contribution will average to zero and so such terms can be neglected. This is known as the rotating wave approximation, and for the example above we then have,

$$H_{RW} = \Omega a^\dagger a + \omega b^\dagger b + \lambda a b^\dagger + \lambda^* a^\dagger b. \quad (3.35)$$

Returning to our exact dynamic, we see then that a general Hamiltonian matrix $K^{(c)}$ in the rotating wave approximation takes the form,

$$K^{(c)} = \begin{pmatrix} 0 & W \\ W & 0 \end{pmatrix}, \quad (3.36)$$

which implies $V = T = \frac{1}{2}W$. Now the creation and annihilation operators decou-

ple in the equations of motion, (3.33), giving,

$$i\dot{A}(t) = WA. \quad (3.37)$$

As a result, we can simplify our numerical analysis greatly, as now our dynamics relies on matrices which are only half the size of those for the full Hamiltonian. Substituting in (3.23) for V and T and taking the matrix exponential leads to³,

$$R(t) = \mathcal{M}R(0) = \begin{pmatrix} T_R & -T_I \\ T_I & T_R \end{pmatrix} R(0). \quad (3.38)$$

where,

$$\begin{aligned} T_R &= \frac{T + T^\dagger}{2} = \cos(Wt), \\ T_I &= \frac{T - T^\dagger}{2i} = -\sin(Wt). \end{aligned} \quad (3.39)$$

The evolution of the covariance matrix can then be found from (3.26).

3.4 Fidelity

Finally, we make some remarks regarding closeness of two Gaussian states. Given ρ_1 and ρ_2 the fidelity between them is defined as $F(\rho_1, \rho_2) = (\text{Tr} \sqrt{\sqrt{\rho_1} \rho_2 \sqrt{\rho_1}})^2$, and is a measure of how close both quantum system are to each other. Actually a distance measure can be defined as $D_B = \sqrt{1 - F}$ which is essentially the same as the Bures distance [84] ($D_{\text{Bures}}^2(\rho_1, \rho_2) = 2 - 2\sqrt{F(\rho_1, \rho_2)}$). This distance will be very useful for quantifying how well the dynamics generated by the Markovian master equations in Chapter 5 approximate the real ones.

In general the fidelity is quite difficult to compute due to the complicated square root factors. However in the case of Gaussian states Scutaru has given closed formulas in terms of the covariance matrix [86]. The key observation is

³For a more explicit derivation, see Section 6.5.1.

that the square root of a Gaussian state is also Gaussian. One then begins by parameterising the characteristic function for desired state $\sqrt{\rho}$ in terms of unknown variables. These can then be determined by relating the terms in the characteristic function of the product, $\chi_{\sqrt{\rho}\sqrt{\rho}}(\xi)$, to the parameters of the characteristic function of the known state, ρ . Repeated application of these techniques allows one to find expressions $\chi_{\sqrt{\rho_1\rho_2}\sqrt{\rho_1}}(\xi)$. Finally, noting $W_0 = 1$ and so $\text{Tr}[O] = \chi_O(0)$, Scutaru was able to give the desired result. In the case of one mode Gaussian states ρ_{G1} and ρ_{G2} , with covariance matrices $\mathcal{C}^{(1)}$ and $\mathcal{C}^{(2)}$ and displacement vectors $\vec{d}^{(1)}$ and $\vec{d}^{(2)}$ respectively, the fidelity is given by the formula

$$F(\rho_{G1}, \rho_{G2}) = \frac{2}{\sqrt{\Lambda + \Phi} - \sqrt{\Phi}} \exp \left[-\delta^T (\mathcal{C}^{(1)} + \mathcal{C}^{(2)})^{-1} \delta \right], \quad (3.40)$$

where $\Lambda = \det [\mathcal{C}^{(1)} + \mathcal{C}^{(2)}]$, $\Phi = \det (\mathcal{C}^{(1)} - 1) \det (\mathcal{C}^{(2)} - 1)$ and $\delta = (\vec{d}^{(1)} - \vec{d}^{(2)})$.

3.5 Summary

In this chapter we have introduced the basic tools needed to handle Gaussian states. In particular, we have shown how the dynamics of a Gaussian system can be efficiently simulated, and under what conditions a Hamiltonian will preserve Gaussian evolution. In later chapters we will apply these techniques in two different contexts. The first as a purely modelling tool, in order to compare the approximate analytic evolution given by a series of master equations to the exact behaviour. While in the second, we extend a class of entropy measures to Gaussian states.

Chapter 4

Markovian Master Equations

4.1 Introduction

It is widely assumed that one of the crucial tasks currently facing quantum theorists is to understand and characterise the behaviour of realistic quantum systems. In any experiment, a quantum system is subject to noise and decoherence due to the unavoidable interaction with its surroundings. The theory of open quantum systems aims at developing a general framework to analyse the dynamical behaviour of systems that, as a result of their coupling with environmental degrees of freedom, will no longer evolve unitarily. If no assumptions are made concerning the strength of the system-environment interaction and the time-correlation properties of the environment, the dynamical problem may become intractable, despite that the functional forms of very general evolutions can be derived [85]. However, there exists a broad range of systems of practical interest, mostly in quantum optics and in solid state physics, where it is possible to account for the observed dynamics by means of a differential equation for the open system's density matrix derived in the context of Markovian processes. Such a differential equation, the so-called Markovian (or Kossakowski-Lindblad) master equation, is required to fulfill several consistency properties such as being trace preserving

and satisfying complete positivity [67, 105, 68, 69, 70, 71, 87, 72].

In the following section we present a brief discussion of how Markovian master equations are obtained in the weak coupling limit (section 4.1.1),

4.1.1 Markovian Master Equations

To derive Markovian Master equations we follow the approach of projection operators initiated by Nakajima [79] and Zwanzig [80], see also [105, 73] for instance. In this method we define in the Hilbert space of the combined system and environment $\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_E$ two orthogonal projection operators, $\mathcal{P}\rho = \text{Tr}_E(\rho) \otimes \rho_E$ and $\mathcal{Q} = \mathbb{I} - \mathcal{P}$, where $\rho \in \mathcal{H}$ is the combined state and $\rho_E \in \mathcal{H}_E$ is a fixed state of the environment, which we choose to be the real initial state, this will be a thermal state $\rho_E = \rho_{\text{th}} = \exp(-H_E/T) \{\text{Tr}[\exp(-H_E/T)]\}^{-1}$. Note that $\mathcal{P}\rho$ gives all the necessary information about the reduced system state ρ_S , so to know the dynamics of $\mathcal{P}\rho$ implies one knows the time evolution of the reduced system.

We then assume that the dynamics of the whole system is given by the Hamiltonian $H = H_S + H_E + \alpha V$, where H_S and H_E are the individual Hamiltonians of system and environment respectively and V describes the interaction between them with coupling strength α . We shall work in the interaction picture, $\tilde{\rho}(t) = \exp[i(H_S + H_E)t]\rho(t)\exp[-i(H_S + H_E)t]$ (and analogously for $\tilde{V}(t)$), thus we obtain the evolution equation

$$\frac{d}{dt}\tilde{\rho}(t) = -i\alpha[\tilde{V}(t), \tilde{\rho}(t)] \equiv \alpha\mathcal{V}(t)\tilde{\rho}(t). \quad (4.1)$$

For the class of interactions in which we are interested $\text{Tr}_E[\tilde{V}(t)\rho_E] = 0$, which implies

$$\mathcal{P}\mathcal{V}(t)\mathcal{P} = 0, \quad (4.2)$$

as can be easily checked by applying it over an arbitrary state $\rho \in \mathcal{H}$. It is not difficult to redefine the interaction Hamiltonian such that this always happens, see for example [72, 77].

Our aim is to obtain a time-evolution equation for $\mathcal{P}\rho$ under some approxi-

mation, in such a way that it describes a quantum Markovian process. To this end, we apply the projection operators on equation (4.1), introducing the identity $\mathbb{I} = \mathcal{P} + \mathcal{Q}$ between $\mathcal{V}(t)$ and $\tilde{\rho}(t)$,

$$\frac{d}{dt}\mathcal{P}\tilde{\rho}(t) = \alpha\mathcal{P}\mathcal{V}(t)\mathcal{P}\tilde{\rho}(t) + \alpha\mathcal{P}\mathcal{V}(t)\mathcal{Q}\tilde{\rho}(t), \quad (4.3)$$

$$\frac{d}{dt}\mathcal{Q}\tilde{\rho}(t) = \alpha\mathcal{Q}\mathcal{V}(t)\mathcal{P}\tilde{\rho}(t) + \alpha\mathcal{Q}\mathcal{V}(t)\mathcal{Q}\tilde{\rho}(t). \quad (4.4)$$

The solution of the second equation can be written formally as

$$\mathcal{Q}\tilde{\rho}(t) = \mathcal{G}(t, t_0)\mathcal{Q}\tilde{\rho}(t_0) + \alpha \int_{t_0}^t ds \mathcal{G}(t, s)\mathcal{Q}\mathcal{V}(s)\mathcal{P}\tilde{\rho}(s),$$

this is nothing but the operational version of the variation of parameters formula for ordinary differential equations (see for example [81, 82]), where the solution to the homogeneous equation

$$\frac{d}{dt}\mathcal{Q}\tilde{\rho}(t) = \alpha\mathcal{Q}\mathcal{V}(t)\mathcal{Q}\tilde{\rho}(t),$$

is given by the propagator

$$\mathcal{G}(t, s) = \mathcal{T}e^{\alpha \int_s^t dt' \mathcal{Q}\mathcal{V}(t')},$$

here $\mathcal{T}$ is the time-ordering operator. Inserting the formal solution for $\mathcal{Q}\tilde{\rho}(t)$ in (4.3) yields

$$\begin{aligned} \frac{d}{dt}\mathcal{P}\tilde{\rho}(t) &= \alpha\mathcal{P}\mathcal{V}(t)\mathcal{P}\tilde{\rho}(t) + \alpha\mathcal{P}\mathcal{V}(t)\mathcal{G}(t, t_0)\mathcal{Q}\tilde{\rho}(t_0) \\ &\quad + \alpha^2 \int_{t_0}^t ds \mathcal{P}\mathcal{V}(t)\mathcal{G}(t, s)\mathcal{Q}\mathcal{V}(s)\mathcal{P}\tilde{\rho}(s). \end{aligned}$$

Since we assume that the initial state is factorized as $\rho(t_0) = \rho_S(t_0) \otimes \rho_{\text{th}}$ we get $\mathcal{Q}\rho(t_0) = 0$ (now we see the advantage of choosing the initial state of the bath

for the definition of the projector $\mathcal{P}$) and using (4.2) we finally find

$$\frac{d}{dt}\mathcal{P}\tilde{\rho}(t) = \int_{t_0}^t ds \mathcal{K}(t, s) \mathcal{P}\tilde{\rho}(s), \quad (4.5)$$

with kernel

$$\mathcal{K}(t, s) = \alpha^2 \mathcal{P}\mathcal{V}(t) \mathcal{G}(t, s) \mathcal{Q}\mathcal{V}(s) \mathcal{P}.$$

The equation (4.5) is still exact, now we perform the weak coupling limit, by taking the kernel at lowest order in α ,

$$\mathcal{K}(t, s) = \alpha^2 \mathcal{P}\mathcal{V}(t) \mathcal{Q}\mathcal{V}(s) \mathcal{P} + \mathcal{O}(\alpha^3), \quad (4.6)$$

so by using again the condition (4.2) we get a Born approximation for (4.5):

$$\frac{d}{dt}\mathcal{P}\tilde{\rho}(t) = \alpha^2 \int_{t_0}^t ds \mathcal{P}\mathcal{V}(t) \mathcal{V}(s) \mathcal{P}\tilde{\rho}(s),$$

which implies

$$\frac{d}{dt}\tilde{\rho}_S(t) = -\alpha^2 \int_{t_0}^t ds \text{Tr}_E[\tilde{V}(t), [\tilde{V}(s), \tilde{\rho}_S(s) \otimes \rho_{\text{th}}]]. \quad (4.7)$$

Now we take the initial time $t_0 = 0$ and an elementary change of variable s by $t - s$ in the integral yields

$$\frac{d}{dt}\tilde{\rho}_S(t) = -\alpha^2 \int_0^t ds \text{Tr}_E[\tilde{V}(t), [\tilde{V}(t - s), \tilde{\rho}_S(t - s) \otimes \rho_{\text{th}}]].$$

We expect this equation to be valid in the limit $\alpha \rightarrow 0$, but in such a limit the change in $\tilde{\rho}_S$ becomes smaller and smaller so if we want to see dynamics we need to rescale the time by a factor α^2 [67, 68, 69] otherwise the right hand of the previous equation goes to zero. So in the limit $\alpha \rightarrow 0$ the integral on the right hand is extended to infinity. However in order to get a finite value for the integral the functions $\text{Tr}_E[\tilde{V}(t), [\tilde{V}(t - s), \rho_B]]$ have to decrease appropriately. Particularly this implies that they should not be periodic, which requires that the number of degrees of freedom in the environment must be infinite, as otherwise

there will be a finite recurrence time. Moreover, as $\tilde{\rho}_S$ changes very slowly in the limit $\alpha \rightarrow 0$, we can take it as a constant inside width τ_B around $s = 0$ where $\text{Tr}_E[\tilde{V}(t), [\tilde{V}(t-s), \rho_B]]$ is not zero, and so finally we obtain

$$\frac{d}{dt}\tilde{\rho}_S(t) = -\alpha^2 \int_0^\infty ds \text{Tr}_E[\tilde{V}(t), [\tilde{V}(t-s), \tilde{\rho}_S(t) \otimes \rho_{\text{th}}]]. \quad (4.8)$$

These informal arguments are just a rough idea behind the rigorous results obtained by Davies [68, 69].

Since we have started from a product state $\rho(t_0) = \rho_S(t_0) \otimes \rho_{\text{th}}$, we require, for consistency, that our evolution equation generates completely positive dynamics. The last equation does not yet warrant complete positivity in the evolution [71], and so we need to perform one final approximation, called the secular approximation. This is, in essence, the rotating wave approximation seen in the last chapter. To this end, note that the interaction Hamiltonian may be written as:

$$V = \sum_k A_k \otimes B_k, \quad (4.9)$$

where each A_k can be decomposed as a sum of eigenoperators of the superoperator $[H_S, \cdot]$

$$A_k = \sum_\nu A_k(\nu), \quad (4.10)$$

where

$$[H_S, A_k(\nu)] = -\nu A_k(\nu). \quad (4.11)$$

This kind of decomposition can always be done [105, 72]. On the other hand, by taking the Hermitian conjugate,

$$[H_S, A_k^\dagger(\nu)] = \nu A_k^\dagger(\nu),$$

and since V is self-adjoint, in the interaction picture one has

$$\tilde{V}(t) = \sum_{\nu,k} e^{-i\nu t} A_k(\nu) \otimes \tilde{B}_k(t) = \sum_{\nu,k} e^{i\nu t} A_k^\dagger(\nu) \otimes \tilde{B}_k^\dagger(t).$$

Now, substituting the decomposition in terms of $A_k(\nu)$ for $\tilde{V}(t-s)$ and $A_k^\dagger(\nu)$ for $\tilde{V}(t)$ into equation (4.8) gives, after expanding the double commutator,

$$\begin{aligned} \frac{d}{dt}\tilde{\rho}_S(t) = & \sum_{\nu,\nu'} \sum_{k,\ell} e^{i(\nu'-\nu)t} \Gamma_{k,\ell}(\nu) [A_\ell(\nu) \tilde{\rho}_S(t), A_k^\dagger(\nu')] \\ & + e^{i(\nu-\nu')t} \Gamma_{k,\ell}^*(\nu) [A_k(\nu'), \tilde{\rho}_S(t) A_\ell^\dagger(\nu)], \end{aligned} \quad (4.12)$$

where we have introduced the quantities

$$\begin{aligned} \Gamma_{k,\ell}(\nu) = & \alpha^2 \int_0^\infty ds e^{i\nu s} \text{Tr} \left[\tilde{B}_k^\dagger(t) \tilde{B}_\ell(t-s) \rho_{\text{th}} \right] \\ = & \alpha^2 \int_0^\infty ds e^{i\nu s} \text{Tr} \left[\tilde{B}_k^\dagger(s) B_\ell \rho_{\text{th}} \right], \end{aligned} \quad (4.13)$$

with the last step being justified because ρ_{th} commutes with $\exp(iH_E t)$.

We can now make the secular approximation. In equation (4.12) the terms with different frequencies will oscillate rapidly around zero as long as $|\nu' - \nu| \gg \alpha^2$, so in the weak coupling limit these terms vanish to obtain,

$$\frac{d}{dt}\tilde{\rho}_S(t) = \sum_{\nu} \sum_{k,\ell} \Gamma_{k,\ell}(\nu) [A_\ell(\nu) \tilde{\rho}_S(t), A_k^\dagger(\nu)] + \Gamma_{k,\ell}^*(\nu) [A_k(\nu), \tilde{\rho}_S(t) A_\ell^\dagger(\nu)]. \quad (4.14)$$

This is justifiable so long as timescale on which the open system changes appreciably is much longer than the typical timescale of the system, i.e. that given by a typical value for $|\nu' - \nu|^{-1}$. As already seen, for quantum optical systems this condition is known as the rotating wave approximation. Now we decompose the matrices $\Gamma_{k,\ell}(\nu)$ as a sum of Hermitian and anti-Hermitian parts

$$\Gamma_{k,\ell}(\nu) = \frac{1}{2} \gamma_{k,\ell}(\nu) + i S_{k,\ell}(\nu),$$

where the coefficients

$$S_{k,\ell}(\nu) = \frac{1}{2i} [\Gamma_{k,\ell}(\nu) - \Gamma_{\ell,k}^*(\nu)],$$

and

$$\gamma_{k,\ell}(\nu) = \Gamma_{k,\ell}(\nu) + \Gamma_{\ell,k}^*(\nu) = \int_{-\infty}^{\infty} ds e^{i\nu s} \text{Tr} \left[\tilde{B}_k^\dagger(s) B_\ell \rho_{\text{th}} \right],$$

form Hermitian matrices. In terms of these quantities (4.14) becomes

$$\frac{d}{dt} \tilde{\rho}_S(t) = -i[H_{\text{LS}}, \tilde{\rho}_S(t)] + \mathcal{D}[\tilde{\rho}_S(t)],$$

where

$$H_{\text{LS}} = \sum_{\nu} \sum_{k,\ell} S_{k,\ell} A_k^\dagger(\nu) A_k(\nu),$$

is a Hermitian operator which commutes with H_S , as a consequence of (4.11). This is usually called the Shift Hamiltonian, since it produces a renormalization of the free energy levels of the system induced by the interaction with the environment. The dissipator is given by

$$\mathcal{D}[\tilde{\rho}_S(t)] = \sum_{\nu} \sum_{k,\ell} \gamma_{k,\ell}(\nu) \left[A_\ell(\nu) \tilde{\rho}_S(t) A_k^\dagger(\nu) - \frac{1}{2} \{ A_k^\dagger(\nu) A_\ell(\nu), \tilde{\rho}_S(t) \} \right].$$

Returning to Schrödinger picture, the time-evolution equation is then just

$$\frac{d}{dt} \rho_S(t) = -i[H_S + H_{\text{LS}}, \rho_S(t)] + \mathcal{D}[\rho_S(t)]. \quad (4.15)$$

Note that the matrices $\gamma_{k,\ell}(\nu)$ are positive semidefinite for every ν . This is a consequence of Bochner's theorem [83], that is, the Fourier transform of a function is positive provided the function is of positive type. It is easy to check that the correlation functions $\text{Tr} \left[\tilde{B}_k^\dagger(s) B_\ell \rho_{\text{th}} \right]$ are functions of positive type, and $\gamma_{k,\ell}(\nu)$ are just the Fourier transform of them, so equation (4.15) can be brought into Lindblad form by diagonalising the coefficient matrix $\gamma(\nu) = (\gamma_{k,\ell}(\nu))$. With this final remark we conclude that the equation (4.15) generates a completely positive semigroup [70] and so defines a proper Markovian master equation.

Chapter 5

Master Equations of Harmonic Oscillator Systems

5.1 Introduction

From the theoretical point of view, the conditions under which Markovian master equations are derived are not always entirely clear, as they generally involve informal approximations motivated by a variety of microscopic models. This leaves open the range of validity of these equations, and which in some circumstances can lead to non physical evolutions. The situation becomes even worse as the complexity of the open system increases. In particular, it is not an easy question to decide whether the dynamics of a composite, possibly driven, quantum system can be described via a Markovian master equation, and if so, in what parameter regime. Indeed, several groups have recently put forward operational criteria to check for deviations from Markovianity of real quantum evolutions [88, 89, 90, 91].

The purpose of this Chapter is to study explicit examples of interacting open quantum systems. In each case, we shall show that there are Markovian master equations which describe the true dynamics very accurately. However, in order to do so it must be possible to efficiently simulate the systems in question, and to this end, we restrict our interest to those consisting of quantum harmonic oscilla-

tors. As we saw in Chapter 3, systems of this type are Gaussian preserving, and so we can easily follow the exact dynamics using numerical simulations. Moreover, this will allow us to test the validity of various mathematical assumptions made in the derivation process and assess their validity. One can then hope the conclusions are general enough to be applicable to non-harmonic systems. In particular, when the coupling between oscillators is sufficiently weak so that their local dynamics is effectively two-dimensional, we expect the conditions obtained for strict Markovianity to be directly applicable to systems of interacting qubits.

The damped harmonic oscillator is the canonical example used in most references to discuss both Markovian and non-Markovian open system dynamics (see for instance [105, 73, 58, 74, 75, 76, 77] and references therein) and exact solutions in the presence of a general environment are known [78]. The dynamics of coupled damped oscillators, including those interacting with a classical field, are significantly less studied, with most analysis focusing on evaluating the decoherence of initially entangled states provided that certain dynamical evolution, Markovian or not, is valid [97]. Recently, an exact master equation for two interacting harmonic oscillators subject to a global general environment was derived [98]. Here we will focus on the derivation of Markovian master equations for interacting systems. We will focus on a scenario where two harmonic systems are subject to independent reservoirs and present a detailed study based on the numerical simulation of the exact dynamics. The advantage of this approach is that it allows us to compute not only quantities for the damped system but also for the environment.

In the following sections we shall study three damped systems. For completeness, the analysis shall begin by considering a single harmonic oscillator (section 5.2) and subsequently move to the core of the study by analyzing the dynamics of two interacting harmonic oscillators (section 5.3), finding Markovian master equations for both weak and strong internal coupling. Finally, we shall address the dynamics of an harmonic oscillator driven by a classical field (section 5.4), where different Markovian master equations can be obtained and studied depending on the values of the external Rabi frequency and the detuning from the oscillator's

natural frequency. To make the reading more fluent, details of the simulations and the derivation procedure are left for the appendices.

5.2 Damped Harmonic Oscillator

We will first consider a single harmonic oscillator damped by an environment consisting of M oscillators (see figure 5.1). We want to know in which conditions the Markovian master equation for the evolution of the damped oscillator is valid. To this aim we will approach the exact dynamical equations of the whole system when M is large; these will be solved via computer simulation, and we can then compare this solution with the one obtained using a master equation.

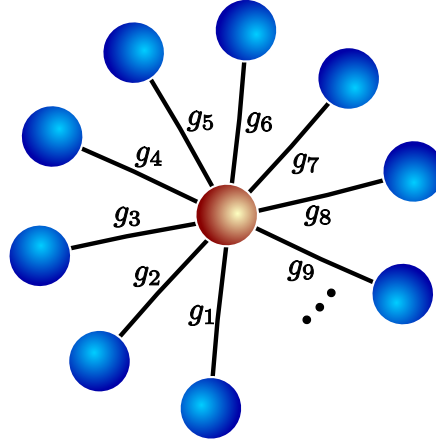


Figure 5.1: Model for a damped harmonic oscillator. The central grey sphere represents the damped oscillator which is coupled to a large number of environmental oscillators (blue spheres) with different frequencies via the coupling constants g_j , which are chosen in agreement with an Ohmic spectral density (5.7).

The Hamiltonian for the whole system will be given by ($\hbar = 1$)

$$H = \Omega a^\dagger a + \sum_{j=1}^M \omega_j a_j^\dagger a_j + \sum_{j=1}^M g_j (a^\dagger a_j + a a_j^\dagger). \quad (5.1)$$

Note that the coupling with the bath has been considered in rotating wave approximation (RWA), which is a good description of the real dynamics for small damping $\Omega \gg \max\{g_j, j = 1, \dots, M\}$ (e.g. in the weak coupling limit).

5.2.1 Markovian Master Equation

The damped harmonic oscillator is a standard example for the derivation of master equations (see for example [105, 74, 75, 77]). It is straightforward to see that the eigenoperators (4.9) of the interaction decompose as,

$$A_1 = A_2^\dagger = a, \quad B_1 = B_2^\dagger = \sum_j^M g_j a_j^\dagger. \quad (5.2)$$

We then proceed by evaluating the elements of (4.13). For the first we have,

$$\Gamma_{1,1}(\Omega) = \sum_{j,j'} g_{1j} g_{j'} \int_0^\infty ds e^{i(\Omega - \omega_j)s} \text{Tr} \left(\rho_B^{\text{th}} a_j a_{j'}^\dagger \right).$$

The bath is assumed to be in a thermal state,

$$\rho_B^{\text{th}} = \frac{\exp -\omega_j a_j^\dagger a_j / T}{\text{Tr}(\exp -\omega_j a_j^\dagger a_j / T)} = \frac{1}{Z} e^{-\omega_j a_j^\dagger a_j / T}, \quad (5.3)$$

and so evaluating the correlation function, we find,

$$\begin{aligned} \Gamma_{1,1}(\Omega) &= \sum_{j=1}^M g_j^2 \int_0^\infty ds e^{i(\Omega - \omega_j)s} \frac{1}{Z} \sum_n e^{-\omega_j n / T} \langle n | a_j^\dagger a_j + [a_j, a_j^\dagger] | n \rangle \\ &= \sum_{j=1}^M g_j^2 \int_0^\infty ds e^{i(\Omega - \omega_j)s} \frac{1}{Z} \sum_n e^{-\omega_j n / T} (n + 1) \\ &= \sum_{j=1}^M g_j^2 \int_0^\infty ds e^{i(\Omega - \omega_j)s} [\bar{n}(\omega_j, T) + 1], \end{aligned} \quad (5.4)$$

where $\bar{n}(\omega, T)$ is the mean number of bath quanta with frequency ω , given by the Bose-Einstein distribution

$$\bar{n}(\omega, T) = \left[\exp \left(\frac{\omega}{T} \right) - 1 \right]^{-1}. \quad (5.5)$$

In Chapter 4, we noted that in order to avoid Poincaré recurrence, the number of oscillators in the bath must tend to infinity. One also requires that their

distribution of frequencies should be smooth. Thus in the expression above, we should take $M \rightarrow \infty$ and replace the summation over oscillator modes by a frequency integral. It is then convenient to introduce the spectral density of the bath as,

$$J(\omega) = \sum_j^M g_j^2 \delta(\omega - \omega_j). \quad (5.6)$$

This function contains information on the frequencies of the modes and their coupling to the system. Indeed, the spectral density completely characterises the heat bath, and for irreversible dynamics we replace $J(\omega)$ by a smooth function of ω . Common choices in the literature are to take the spectral density to be proportional to some power of ω , $J(\omega) \sim \alpha \omega^s$ for small frequencies. There are then three standard regimes, known as Ohmic, sub-Ohmic and super-Ohmic, corresponding to $s = 1$, $s < 1$ and $s > 1$ respectively¹. The Ohmic case is by far the most well understood, in part due to its importance in early phenomenological studies, but also because of its comparative analytical convenience. In practice however, it is not an entirely realistic model as the spectral density diverges for high frequencies. To account for this we introduce a suitable high-frequency cutoff. This can be done in many ways, and the particular choice will usually depend on the specific application. For systems where the physical frequencies are much less than the cut off frequency however, this choice is largely unimportant, leading only to a renormalising of the parameters in the system Hamiltonian. For definiteness, in this thesis we have chosen to distribute the environmental oscillators according to an Ohmic spectral density, with exponential cutoff [76]

$$J(\omega) = \sum_j^M g_j^2 \delta(\omega - \omega_j) \rightarrow \alpha \omega e^{-\omega/\omega_c}, \quad (5.7)$$

where α is a constant which modifies the strength of the interaction and ω_c is the so-called cutoff frequency. Clearly $J(\omega)$ increases linearly for small values of ω , decays exponentially for large ones, and has its maximum at $\omega = \omega_c$.

¹Historically this naming convention can be traced back to modelling dissipation in LCR circuits.

Returning to equation (5.4), the time integral can be evaluated by making use of the formula,

$$\int_0^\infty ds e^{i\epsilon s} = \pi\delta(\epsilon) - i\text{P.V.}\frac{1}{\epsilon}, \quad (5.8)$$

where P.V. denotes the Cauchy principal value of the integral. Now on substituting our choice of spectral density (5.7) we find the Markovian master equation (4.15) is given by

$$\begin{aligned} \frac{d}{dt}\rho(t) = & -i\bar{\Omega}[a^\dagger a, \rho(t)] + \gamma(\bar{n} + 1) (2a\rho(t)a^\dagger - a^\dagger a\rho(t) - \rho(t)a^\dagger a) \\ & + \gamma\bar{n} (2a^\dagger \rho(t)a - aa^\dagger \rho(t) - \rho(t)aa^\dagger). \end{aligned} \quad (5.9)$$

Here $\bar{n} = \bar{n}(\Omega, T)$ and γ is the decay rate,

$$\gamma = \pi J(\Omega), \quad (5.10)$$

In addition the oscillator energy Ω in the first term is renormalised (Lamb shifted) $\bar{\Omega}$ due to the coupling with the high frequency modes of the environment:

$$\bar{\Omega} = \Omega + \Delta, \quad \Delta = \text{P.V.} \int_0^\infty d\omega \frac{J(\omega)}{\Omega - \omega}, \quad (5.11)$$

Note that this shift Δ is independent of the temperature, and although its effect is typically small (e.g. [105, 75]) we will not neglect it in our study. For an Ohmic spectral density the shift in the frequency is

$$\Delta = \alpha \text{P.V.} \int_0^\infty d\omega \frac{\omega e^{-\omega/\omega_c}}{\Omega - \omega} = \alpha \Omega e^{-\Omega/\omega_c} \text{Ei}(\Omega/\omega_c) - \alpha \omega_c,$$

where Ei is the exponential integral function defined as

$$\text{Ei}(x) = -\text{P.V.} \int_{-x}^\infty \frac{e^{-t}}{t} dt.$$

In addition, note that the equation (5.9) preserves the Gaussian character of the states [92].

5.2.2 Simulating the exact solution

In order to assess how well (5.9) performs, we must also simulate the exact solution of the system in order that appropriate comparisons can be made. This requires two ingredients. The first involves solving the complete dynamical equations of the system, from which the evolution of the test oscillator can be found by tracing out the bath. On their own, however, these equations do not provide the relevant insight into the expected dynamics because the Hamiltonian specified in (5.1) is still too general. In order to correspond to a realistic physical situation, we must also include some assumptions about the bath, and in particular this means specifying how we choose the parameters ω_j and g_j .

Exact dynamical equations

The exact solution for the evolution of system is most easily given in terms of the time-evolution of the collection of annihilation operators $\{a, a_j\}$. From (5.1) we have

$$i\dot{a} = [a, H] = \Omega a + \sum_{j=1}^M g_j a_j, \quad (5.12)$$

$$i\dot{a}_j = [a_j, H] = \omega_j a_j + g_j a, \quad (5.13)$$

and so by writing $A = (a, a_1, a_2, \dots, a_M)^T$, the system of differential equations may be expressed as

$$i\dot{A} = WA, \quad (5.14)$$

where W is the matrix

$$W = \begin{pmatrix} \Omega & g_1 & g_2 & \cdots & g_M \\ g_1 & \omega_1 & & & \\ g_2 & & \omega_2 & & \\ \vdots & & & \ddots & \\ g_M & & & & \omega_M \end{pmatrix}. \quad (5.15)$$

Now, noting that the linearity in the couplings in H imply that an initial (global) Gaussian state ρ_G will remain Gaussian at all times t (Section 3.3), and so we can restrict our attention to the evolution of its covariance matrix, $\mathcal{C}$,

$$\mathcal{C}_{i,j} = \langle R_i R_j + R_j R_i \rangle - 2\langle R_i \rangle \langle R_j \rangle. \quad (5.16)$$

From Section 3.3.2 we have,

$$\mathcal{C}(t) = \mathcal{M}\mathcal{C}(0)\mathcal{M}^T, \quad (5.17)$$

where $\mathcal{M}$ is a $2(M+1) \times 2(M+1)$ matrix given by,

$$\begin{aligned} \mathcal{M} &= \begin{pmatrix} T_R & -T_I \\ T_I & T_R \end{pmatrix}; \\ T_R &= \frac{T + T^\dagger}{2} = \cos(Wt), \\ T_I &= \frac{T - T^\dagger}{2i} = -\sin(Wt). \end{aligned} \quad (5.18)$$

In order to simplify the simulations further, we note that in most cases we are only interested in the behaviour of the subsystem comprising of the test oscillator a . All the information pertaining to it's dynamical evolution is contained in the 2×2 submatrix $\{\mathcal{C}_{ij}; i, j = 1, M+2\}$. Writing out the elements of covariance matrix, we have

$$\mathcal{C}_{i,j}(t) = \sum_{k,\ell} \mathcal{M}_{i,k} \mathcal{M}_{j,\ell} \mathcal{C}_{k,\ell}(0), \quad (5.19)$$

and so we can calculate the submatrix above from the following,

$$\begin{aligned} \mathcal{C}_{1,1}(t) &= \sum_{k,\ell} \mathcal{M}_{1,k} \mathcal{M}_{1,\ell} \mathcal{C}_{k,\ell}(0) = (\mathcal{M}_1, \mathcal{C} \mathcal{M}_1), \\ \mathcal{C}_{1,M+2}(t) &= \mathcal{C}_{M+2,1}(t) = \sum_{k,\ell} \mathcal{M}_{1,k} \mathcal{M}_{M+2,\ell} \mathcal{C}_{k,\ell}(0) = (\mathcal{M}_1, \mathcal{C} \mathcal{M}_{M+2}), \\ \mathcal{C}_{M+2,M+2}(t) &= \sum_{k,\ell} \mathcal{M}_{M+2,k} \mathcal{M}_{M+2,\ell} \mathcal{C}_{k,\ell}(0) = (\mathcal{M}_{M+2}, \mathcal{C} \mathcal{M}_{M+2}), \end{aligned} \quad (5.20)$$

here $(\cdot, \cdot)$ denotes the scalar product, and the vectors $\mathcal{M}_1$ and $\mathcal{M}_{M+2}$ are

$$\begin{aligned}\mathcal{M}_1 &= (\mathcal{M}_{1,1}, \mathcal{M}_{1,2}, \dots, \mathcal{M}_{1,2M+2})^T, \\ \mathcal{M}_{M+2} &= (\mathcal{M}_{M+2,1}, \mathcal{M}_{M+2,2}, \dots, \mathcal{M}_{M+2,2M+2})^T.\end{aligned}\tag{5.21}$$

Spectral Density of the Bath

The final ingredient is to make a careful choice of a number numerical parameters involved in the simulation. In practice, however, this is not a potentially difficult issue. The essential requirement is to choose the couplings to bath according to the desired spectral density. While many choices are available, in this thesis we will consistently assume an Ohmic spectral density (5.7). The first step in choosing g_j is to remove the Dirac delta functions by integrating over a frequency range bounded by a frequency cut-off $\omega_{\max}$,

$$\sum_j g_j^2 \approx \alpha \int_0^{\omega_{\max}} \omega e^{-\omega/\omega_c} d\omega,$$

which means

$$g_{j'}^2 \approx \alpha \omega_{j'} e^{-\omega_{j'}/\omega_c} \Delta\omega_{j'},$$

due to the decomposition of the integral in terms of Riemann sums. Here $\Delta\omega_{j'}$ is the frequency spacing between oscillators (typically $\omega_{\max}/M$ in our simulations). We should also take care to set the range of oscillators, $\omega_{\max}$, large enough to cover (5.7) significantly. For example, if we take $\omega_1 = c$, with c small, then one possible convention is to take $\omega_{\max}$ such that $J(\omega_{\max}) = J(c)$, and so we neglect all possible oscillators with coupling constant less than $\sqrt{J(c)\Delta\omega_1}$. Another convention would be to take ω_1 and $\omega_{\max}$ such that

$$\begin{aligned}\int_0^{\omega_1} J(\omega) d\omega &= \int_{\omega_{\max}}^{\infty} J(\omega) d\omega \\ \Rightarrow \omega_c - e^{-\omega_1/\omega_c}(\omega_1 + \omega_c) &= (\omega_{\max} + \omega_c)e^{-\omega_{\max}/\omega_c}.\end{aligned}$$

In practice, however, this choice is not a crucial point and unless otherwise specified we take our cutoff frequency and range to be $\omega_c = 3$ and $\omega_{\max} = 20$

5.2.3 Study of the Approximations

We now begin our assessment of the Markovian master equation (5.9). This equation has been extensively studied in the literature, however here our motivation is to test a number of effects pertaining to the general validity of such derivations. This will act as a grounding for later sections, where the master equations necessarily rely on stronger assumptions. In particular, we shall look at three issues. The first concerns the validity of the simulations themselves when we are restricted to modelling a finite bath. While the second and third relate to assumptions made in the derivation process itself. As an initial informative check, in figure 5.2 we plot the variance of the x coordinate for two different initial states of the system, a thermal and a squeezed state. The last plot clearly illustrates the accuracy of the master equation, when compared to the effect of the Lamb shift. To explore this further, we now study several effects which attain to the validity Equation (5.9). Throughout we make our comparisons by calculating the fidelity between the simulated state $\rho_S^{(s)}$ and the state generated by the master equation $\rho_S^{(m)}$.

Discreteness of the bath

Due to the finite number of oscillators in the bath, we can only simulate inside of a bounded time scale free of the back-action of the bath. This produces revivals in the visualized dynamical quantities for times $t < \tau_R$, where τ_R is the recurrence time of the bath. Of course the time at which these revivals arise increases with the number of oscillators in the bath, and roughly speaking it scales as $\tau_R \propto M$. This behaviour is shown in figure 5.3, where the distance between the simulation and the master equation for a system initially in a thermal state with temperature $T_S = 30$ is plotted as a function of the time and the number of oscillators.

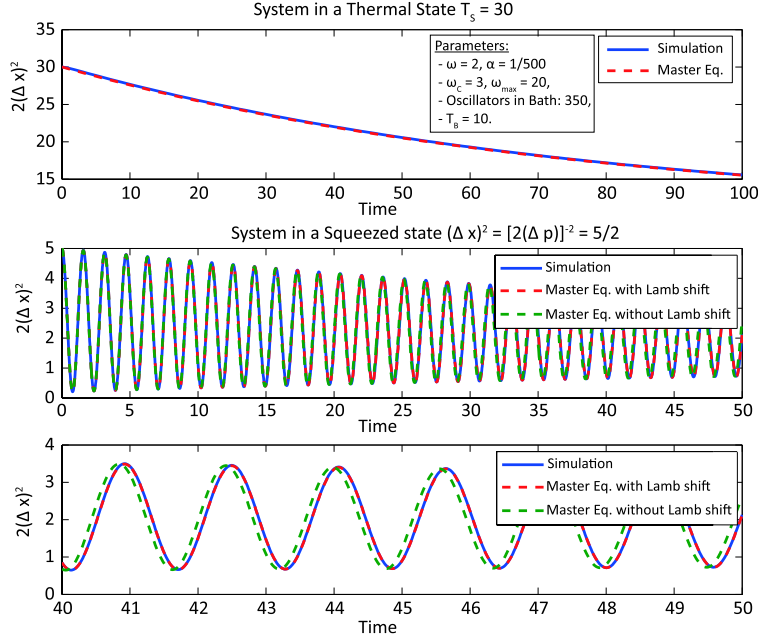


Figure 5.2: Comparison of the evolution of $2(\Delta x)^2$ for an initially thermal and squeezed (vacuum) state and effect of the Lamb shift.

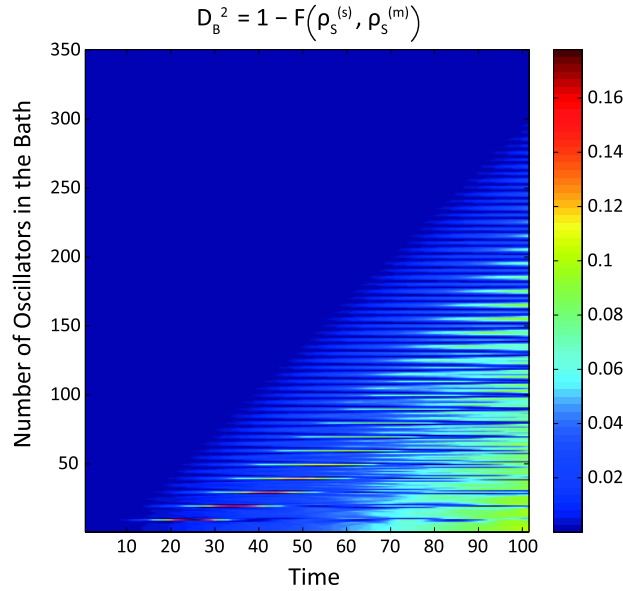


Figure 5.3: Colour map showing the dependency of the recurrence times with the size of the bath. The rest of parameters are the same as figure 5.2.

Temperature

It is sometimes claimed that for ohmic spectral densities the master equation (5.9) is not valid at low temperatures [75, 76]. Of course, one must make clear the context in which this claim is made, and so for definiteness, let us focus on the validity with respect to the bath temperature. A detailed discussion of this situation can be found in the book by Carmichael [75]. There the argument is based on the width of the correlation function $C_{12}(\tau) = \text{Tr}[\tilde{B}_1(s)B_2\rho_{\text{th}}]$, where $B_1^\dagger = B_2 = \sum_{j=1}^M g_j a_j$, which increases for an Ohmic spectral density as the bath temperature decreases. More specifically, in the derivation of the master equation two kinds of correlation functions appear, these are

$$\begin{aligned} C_{12}(s) &= \text{Tr}[\tilde{B}_1(s)B_2\rho_{\text{th}}] = \sum_{j,k} g_k g_j e^{i\omega_j s} \text{Tr}[a_j^\dagger a_k \rho_{\text{th}}] \\ &= \sum_j^M g_j^2 e^{i\omega_j s} \bar{n}(\omega_j, T), \end{aligned}$$

and

$$\begin{aligned} C_{21}(s) &= \text{Tr}[\tilde{B}_2(s)B_1\rho_{\text{th}}] = \sum_{j,k} g_k g_j e^{-i\omega_j s} \text{Tr}[a_j a_k^\dagger \rho_{\text{th}}] \\ &= \sum_j^M g_j^2 e^{-i\omega_j s} [\bar{n}(\omega_j, T) + 1]. \end{aligned}$$

We may call $C_{12}(s) \equiv C(-s, T)$ and $C_{21}(s) \equiv C(s, T) + C_0(s)$, and so in the continuous limit

$$C_0(s) = \int_0^\infty J(\omega) e^{-i\omega s} d\omega = \alpha \int_0^\infty \omega e^{-i\omega(s-\omega_c^{-1})} d\omega = \frac{\alpha \omega_c^2}{(is\omega_c + 1)^2},$$

and

$$C(s, T) = \int_0^\infty J(\omega) e^{-i\omega s} \bar{n}(\omega, T) d\omega = \alpha T^2 \zeta\left(2, 1 - isT + \frac{T}{\omega_c}\right),$$

where here $\zeta(z, q) = \sum_{k=0}^\infty \frac{1}{[(q+k)^2]^{z/2}}$ is the so-called Hurwitz Zeta function, which is a generalization of the Riemann zeta function $\zeta(z) = \zeta(z, 1)$ [94].

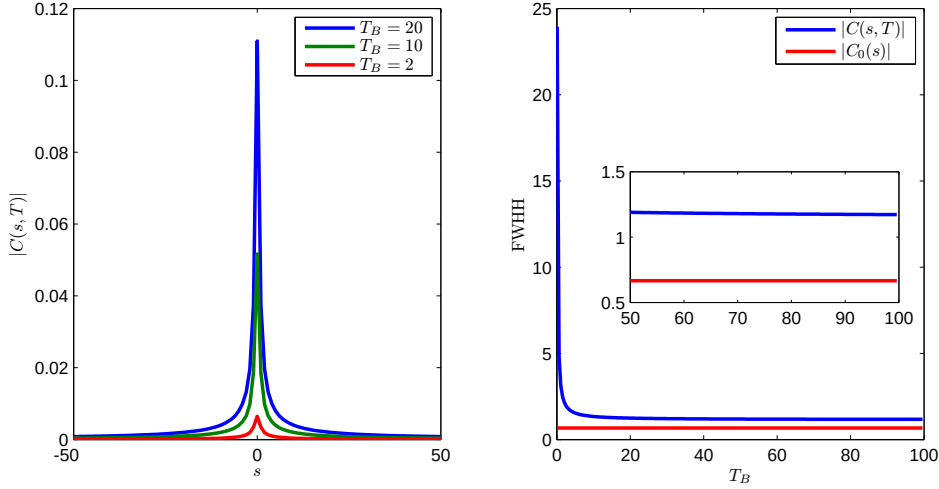


Figure 5.4: On the left, the absolute value of the correlation function is plotted for several temperatures while the FWHH as a function of the temperature is represented on the right hand.

In the left plot of figure 5.4, the absolute value of $C(s, T)$ is plotted for different temperatures. Note that the spreading of the correlation function is mainly caused by its “height” decrease, that is, in the limit $T \rightarrow 0$, $C(s, T) \rightarrow 0$. So one may also expect that the contribution of these correlations to the motion becomes less important as $T \rightarrow 0$, in such a way that the problem of the infinite width can be counteracted, and this is indeed what seems to happen. To visualize this more carefully we have plotted in the right hand of figure 5.4 the full weight at half height (FWHH) for both $C_0(s)$ and $C(s, T)$. In order to make valid the Markovian approximation, the typical time scale for the evolution of the system due to its interaction with the bath τ_S , must be large in comparison with the decay time τ_B of the correlation functions. Loosely speaking, this can be characterized by the FWHH.

From figure 5.4 one sees that for small temperatures τ_B (i.e. FWHH) is quite large, so it is expected that the Markovian approximation breaks down for values of T such that $\tau_S \lesssim \tau_B$. However if α is small enough this will happen for values where the contribution of $C(s, T)$ to the convolution integrals is negligible in comparison with the contribution of $C_0(s)$, whose FWHH will remain constant

and small with respect to τ_S . As a rough estimation, using the parameters in figure 5.2, we find that to get a value of the FWHH comparable with $\tau_S \sim 1/\sqrt{\alpha} \sim 22.4$, we need a temperature of at least $T \sim 0.05$. Both contributions enter in the Markovian master equation derivation via some convolution with the quantum state and one oscillating factor. We may get a very informal idea of how both contributions matter by looking at their maximum values at $s = 0$, for example $C(s = 0, T = 0.05) = 3.27391 \times 10^{-7}$ and $C_0(s = 0) = 0.018$, and so it is clear that $C(s, T = 0.05)$ will not have a large effect on the dynamics. For large temperatures the FWHH of $C(s, T)$ remains small though now larger than $C_0(s)$, so it is expected that in the limit of high temperatures the accuracy of the Markovian master equation stabilizes to a value only a little worse than for $T = 0$.

All of these conclusions are illustrated in figure 5.5, where the fidelity between the state from the simulation and that from the Markovian master equation is plotted. The behaviour at very early times is mainly related to the choice of the initial state of the system, and reflects how it adjusts to the state of the bath under the Markovian evolution [95], different tendencies have been found depending on the choice of initial state. However the behaviour with temperature is visible at longer times (since $\tau_B \sim \text{FWH}$ increases with T) which is in agreement with the conclusions drawn from the correlation functions (see small subplot). At zero temperature (blue line) the results are in closest agreement, however, as the temperature is increased to $T = 0.1$ the correlation function broadens, which leads to a degradation (albeit small) in the modelling precision. As the temperature increases further, the influence of this correlation function becomes more important and the FWHH decreases to a limiting value (see the plot on the right of figure 5.4), this convergence is reflected by the red, cyan and purple lines which show that the accuracy at large temperatures stabilizes to only a little worse than that at $T = 0$, as was expected from figure 5.4.

In summary, the master equation (5.9) does not properly describe the stimulated emission/absorption processes (the ones which depend on $C(s, T)$) for low temperatures, however the temperatures when this discrepancy is apparent are so

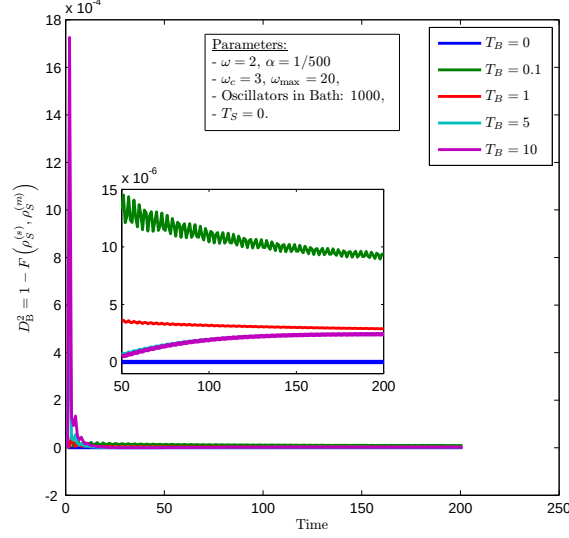


Figure 5.5: Fidelity between the simulated state ρ_S and that given by the master equation time evolution ρ_M , for several temperatures.

small that the contribution from stimulated process are negligible in comparison with spontaneous emission, and the master equation will still give good results.

Assumption of factorized dynamics $\rho(t) = \rho_S(t) \otimes \rho_{th}$

In the derivation of the master equation, one can arrive at equation (4.7) by iterating the Von-Neumann equation (4.1) twice and assuming that the whole state factorizes as $\rho(t) \approx \rho_S(t) \otimes \rho_{th}$ at any time ([105, 72, 75, 77]). This assumption has to be understood as an effective model for arriving at equation (4.7) without using the projection operator techniques, but it does not make sense to assume that the physical state of the system is a factorization for all time. Taking advantage of the ability to simulate the entire system we have plotted the distance between the simulated whole state $\rho(t)$ and the ansatz $\rho_S(t) \otimes \rho_{th}$ as a function of the time, see figure 5.6. On the left side the distance is plotted for $M = 350$ oscillators in bath, actually we have checked from several simulations the results turn out to be independent of the number of oscillators as long as the maximum time in the plot is smaller than the recurrence time of the system. Since $t = 50$ is less than the recurrence time for $M = 175$ (see figure 5.3) we have used this value

and plotted the distance for different coupling strengths on the right. It is clear

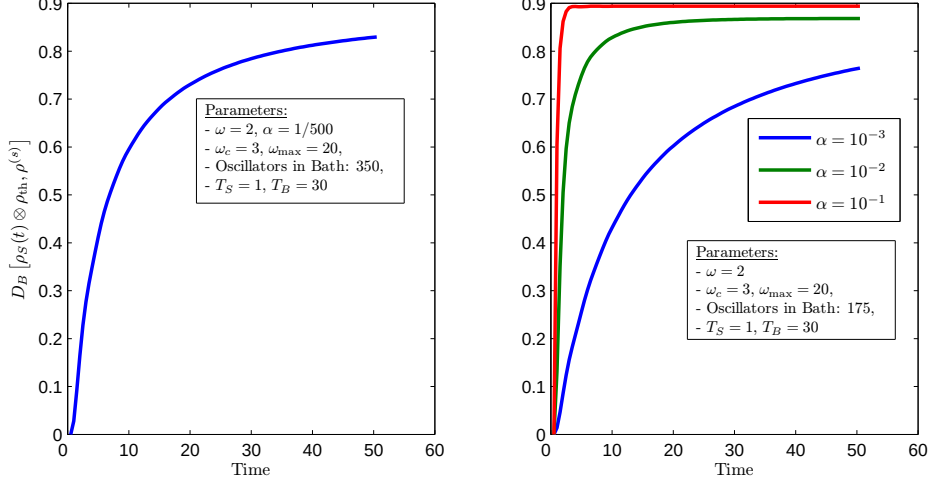


Figure 5.6: Distance between the simulated states $\rho_S(t) \otimes \rho_{th}$ and $\rho(t)$ as a function of time, on the left side different number of oscillators in bath are plotted (obtaining the same result on that time scale) and on the right side different values of the coupling constant has been taken.

that this distance is monotonically increasing in time (strictly, in the limit of an environment with infinite degrees of freedom), and the slope decreases with coupling strength. In section 4.1.1 we pointed out that the weak coupling approach make sense if the coupling is small and the environment has infinite degrees of freedom. This fits with the usual argument to take $\rho \approx \rho_S(t) \otimes \rho_{th}$, that is “the state of the environment is not so affected by the system” in those more informal derivation of Markovian master equations, but we stress again that this is an effective approach, without any physical meaning on the real state ρ .

5.3 Two Coupled Damped Harmonic Oscillator

We now consider two coupled harmonic oscillators, which for simplicity we take to have the same frequency $\Omega_1 = \Omega_2 = \Omega$, and each locally damped by their own reservoir (see figure 5.7), the Hamiltonian of the whole system is

$$H = H_{01} + H_{02} + V_{12} + H_{B1} + H_{B2} + V_{1B1} + V_{2B2}, \quad (5.22)$$

where the free Hamiltonians are given by

$$\begin{aligned} H_{01} &= \Omega a_1^\dagger a_1, & H_{02} &= \Omega a_2^\dagger a_2, \\ H_{B1} &= \sum_{j=1}^M \omega_{1j} a_{1j}^\dagger a_{1j}, & H_{B2} &= \sum_{j=1}^M \omega_{2j} a_{2j}^\dagger a_{2j}, \end{aligned}$$

with the couplings to the baths,

$$\begin{aligned} V_{1B1} &= \sum_{j=1}^M g_{1j} (a_1^\dagger a_{1j} + a_1 a_{1j}^\dagger), \\ V_{2B2} &= \sum_{j=1}^M g_{2j} (a_2^\dagger a_{2j} + a_2 a_{2j}^\dagger), \end{aligned}$$

and the coupling between oscillators,

$$V_{12} = \beta (a_1^\dagger a_2 + a_1 a_2^\dagger).$$

Again we have employed the rotating wave approximation, and so we assume $\Omega \gg \beta$. In the case of $\Omega \sim \beta$ we must keep the antirotating terms $a_1 a_2$ and $a_1^\dagger a_2^\dagger$, note however that the eigenfrequencies of the normal modes become imaginary if $\omega < 2\beta$ (see for example [93]), and so even when keeping the antirotating terms, we must limit β if we wish to keep the oscillatory behaviour.

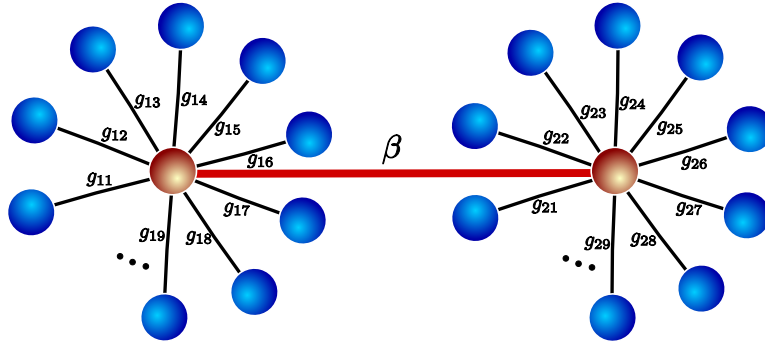


Figure 5.7: The same model as figure 5.1 for the case of two damped harmonic oscillators coupled between them with strength β .

5.3.1 Exact Solution

For the exact solution, the extension to two oscillators follows closely that of a single damped harmonic oscillator. Again, we work in the Heisenberg picture, and wish to solve for the vector $A = (a_1, a_{11}, \dots, a_{1M}, a_2, a_{21}, \dots, a_{2M})^T$, given the differential equation,

$$i\dot{A} = WA, \quad (5.23)$$

where W is now given by the matrix

$$W = \begin{pmatrix} \Omega_1 & g_{11} & \cdots & g_{1M} & \beta & & & \\ & g_{11} & \omega_{12} & & & & & \\ & \vdots & & \ddots & & & & \\ & g_{1M} & & & \omega_{1M} & & & \\ \beta & & & & & \Omega_2 & g_{21} & \cdots & g_{2M} \\ & & & & & g_{21} & \omega_{21} & & \\ & & & & & \vdots & & \ddots & \\ & & & & & g_{2M} & & & \omega_{2M} \end{pmatrix}. \quad (5.24)$$

The simulation process is then analogous to that of section 5.2.2.

5.3.2 Markovian Master Equations

Unfortunately, the derivation of a master equation for coupled systems introduces a number of additional complications. If the oscillators are uncoupled $\beta = 0$, it is obvious that the master equation for their joint density matrix will be a sum of expressions like (5.9),

$$\frac{d}{dt}\rho_S(t) = -i[\bar{\Omega}a_1^\dagger a_1 + \bar{\Omega}a_2^\dagger a_2, \rho_S(t)] + \mathcal{D}_1[\rho_S(t)] + \mathcal{D}_2[\rho_S(t)], \quad (5.25)$$

where

$$\begin{aligned}\mathcal{D}_j[\rho_S(t)] = & \gamma_j(\bar{n}_j + 1) \left(2a_j\rho_S(t)a_j^\dagger - a_j^\dagger a_j \rho_S(t) - \rho_S(t)a_j^\dagger a_j \right) \\ & + \gamma_j\bar{n}_j \left(2a_j^\dagger \rho_S(t)a_j - a_j a_j^\dagger \rho_S(t) - \rho_S(t)a_j a_j^\dagger \right),\end{aligned}\quad (5.26)$$

here each frequency shift, decay rate and number of quanta are individually computed via equations (5.5), (5.10) and (5.11) for each bath j . However for finite intercoupling we split the analysis in two subsections.

Small intercoupling β

If β is small enough to not effect the shift and decay rates, one can expect a master equation of the form

$$\frac{d}{dt}\rho_S(t) = -i[\bar{\Omega}a_1^\dagger a_1 + \bar{\Omega}a_2^\dagger a_2 + V_{12}, \rho_S(t)] + \mathcal{D}_1[\rho_S(t)] + \mathcal{D}_2[\rho_S(t)], \quad (5.27)$$

an example of this for coupled subsystems can be found in [96], and we have detailed a derivation based in projection operators in 5.A.1. In addition this kind of approximation is often made in other contexts such as with damped systems driven by a classical field [75]. Such a case will be analyzed in detail in section 5.4.

Large intercoupling β

To go further in deriving a master equation for a pair of coupled damped oscillators, we must work in the interaction picture generated by the Hamiltonian $H_0 = H_{\text{free}} + V_{12}$ and apply the procedure described in section 4.1.1.

The details of the derivation are left for 5.A.2, what is important however, is that the non-secular terms oscillate with a phase $e^{\pm 2i\beta t}$ so in order to neglect them we have to impose $\beta \gg \alpha$, therefore the resultant equation is, in some sense, complementary to (5.27) valid if $\alpha \gtrsim \beta$. The final master equation in this regime takes the form

$$\begin{aligned}
\frac{d}{dt}\rho_S(t) = & -i[\bar{\Omega}a_1^\dagger a_1 + \bar{\Omega}a_2^\dagger a_2 + \bar{\beta}(a_1a_2^\dagger + a_1^\dagger a_2), \rho_S(t)] \\
& + \sum_{j,k}^2 K_{jk}^{(E)} \left[a_j \rho_S(t) a_k^\dagger + \frac{1}{2} \{a_k^\dagger a_j, \rho_S(t)\} \right] \\
& + \sum_{j,k}^2 K_{jk}^{(A)} \left[a_j^\dagger \rho_S(t) a_k + \frac{1}{2} \{a_k a_j^\dagger, \rho_S(t)\} \right], \tag{5.28}
\end{aligned}$$

here

$$\begin{aligned}
\bar{\Omega} &= \Omega + [\Delta_1(\Omega_+) + \Delta_2(\Omega_+) + \Delta_1(\Omega_-) + \Delta_2(\Omega_-)]/4, \\
\bar{\beta} &= \beta + [\Delta_1(\Omega_+) + \Delta_2(\Omega_+) - \Delta_1(\Omega_-) - \Delta_2(\Omega_-)]/4,
\end{aligned}$$

and $K_{jk}^{(E)}$ and $K_{jk}^{(A)}$ are two positive semidefinite Hermitian matrices with coefficients

$$\begin{aligned}
K_{11}^{(E)} = K_{22}^{(E)} = & \{ \gamma_1(\Omega_+) [\bar{n}_1(\Omega_+) + 1] + \gamma_2(\Omega_+) [\bar{n}_2(\Omega_+) + 1] \\
& + \gamma_1(\Omega_-) [\bar{n}_1(\Omega_-) + 1] + \gamma_2(\Omega_-) [\bar{n}_2(\Omega_-) + 1] \} / 2, \tag{5.29}
\end{aligned}$$

$$\begin{aligned}
K_{12}^{(E)} = K_{21}^{(E)*} = & \{ \gamma_1(\Omega_+) [\bar{n}_1(\Omega_+) + 1] + \gamma_2(\Omega_+) [\bar{n}_2(\Omega_+) + 1] \\
& - \gamma_1(\Omega_-) [\bar{n}_1(\Omega_-) + 1] - \gamma_2(\Omega_-) [\bar{n}_2(\Omega_-) + 1] \} / 2, \tag{5.30}
\end{aligned}$$

$$\begin{aligned}
K_{11}^{(A)} = K_{22}^{(A)} = & [\gamma_1(\Omega_+) \bar{n}_1(\Omega_+) + \gamma_2(\Omega_+) \bar{n}_2(\Omega_+) \\
& + \gamma_1(\Omega_-) \bar{n}_1(\Omega_-) + \gamma_2(\Omega_-) \bar{n}_2(\Omega_-)] / 2, \tag{5.31}
\end{aligned}$$

$$\begin{aligned}
K_{12}^{(A)} = K_{21}^{(A)*} = & [\gamma_1(\Omega_+) \bar{n}_1(\Omega_+) + \gamma_2(\Omega_+) \bar{n}_2(\Omega_+) \\
& - \gamma_1(\Omega_-) \bar{n}_1(\Omega_-) - \gamma_2(\Omega_-) \bar{n}_2(\Omega_-)] / 2, \tag{5.32}
\end{aligned}$$

where γ_j , Δ_j and $\bar{n}_j$ are evaluated according to the spectral density and temperature of the bath j and $\Omega_\pm = \Omega \pm \beta$.

5.3.3 Study of the Approximations

By virtue of the derivation, equations (5.27) and (5.28) preserve both complete positivity and Gaussianity. Thus we can test their regimes of validity using simulations of Gaussian states, and the appropriate fidelity formulas. In figure 5.8 we have plotted the fidelity between both states for the master equation (5.27) (left side) and for (5.28) (right side).

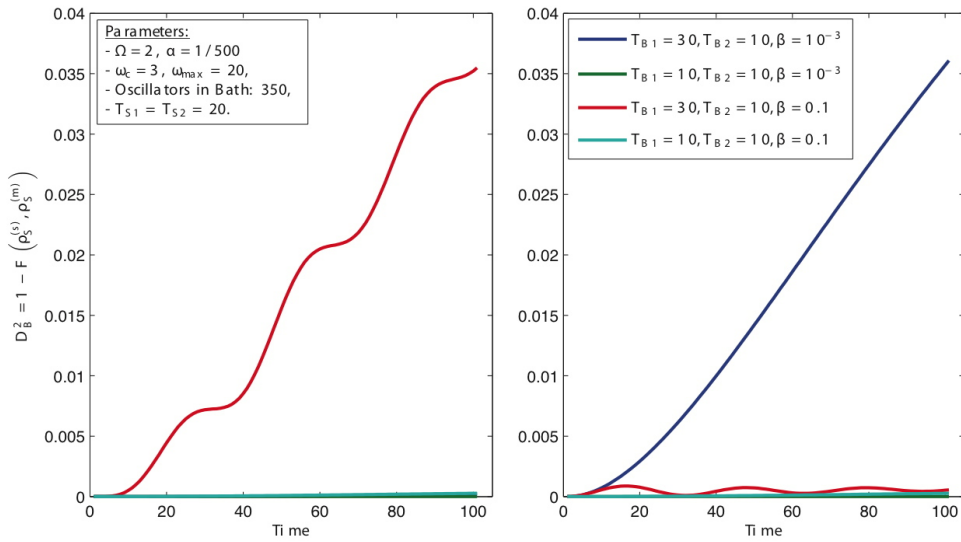


Figure 5.8: On the left, the fidelity between the simulated state $\rho_S^{(s)}$ and that according to the master equation (5.27). The analog using equation (5.28) is plotted on the right. In both plots the parameters and legends are the same.

From these results one concludes that when modeling a system with multiple baths at different temperatures equations (5.27) and (5.28) are each accurate in their theoretically applicable regimes. However, for baths at the same temperature, it seems both equations give good results. A natural, and important, question is to ask is whether an intermediate range of couplings exist, such that neither (5.27) or (5.28) give useful results. In figure 5.9 the fidelity between the simulation and the master equation states have been plotted for both equations at fixed time $t = 100$ as a function of the intercoupling strength β .

We see that for the parameters shown on the plot, there is a small range

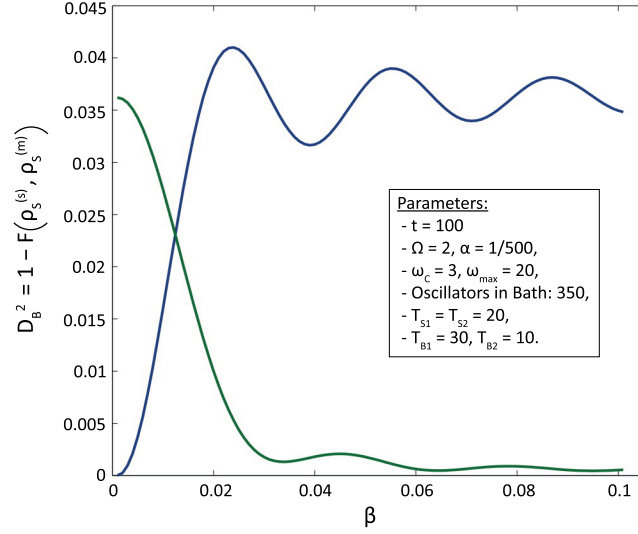


Figure 5.9: Fidelity between the simulated state $\rho_S^{(s)}$ and the ones $\rho_S^{(m)}$ according to the master equations (5.27) (blue) and (5.28) (green) at fixed time as a function of the coupling between damped oscillators.

between $\beta \sim 0.01 - 0.02$ where neither master equation obtains a high precision. However, note that this range becomes smaller as the coupling with the bath decreases, and so generally both master equations cover a good range of values of β .

Baths with the same temperature

We now examine the role of the bath temperatures in more detail. Since the simulation seems to produce good results for both master equations when the temperature of the local baths are the same, regardless of the strength of the intercoupling, it is worth looking at why this happens. In the case of equation (5.28) it is reasonable to expect that this will remain valid for low β , as when $\beta \rightarrow 0$ this equation approaches (5.27) if the bath temperatures and spectral densities are the same. That is, the off-diagonal terms of the matrices $K^{(E)}$ and $K^{(A)}$ do not contribute much, $\bar{\beta} \sim \beta$ and the rest of coefficients become approximately equal to those in (5.27). Note that this only happens under these conditions.

Essentially the same argument applies to equation (5.27) in the large β limit. On the one hand, for a relatively small value of β ($= 0.1$) in comparison to ω , the off-diagonal elements of the matrices $K^{(E)}$ and $K^{(A)}$ in the master equation (5.28) are unimportant in comparison with the diagonals. On the other hand, the diagonal terms are also similar for the same reason, and so both master equations will be quite similar. However note that at later times the behaviour of both equations start to differ, and the steady states are not the same. By construction, the steady state of equation (5.28) is the thermal state of the composed system [105, 68], whereas that of master equation (5.27) is not (although it tends to the thermal state as $\beta \rightarrow 0$ of course). Surprisingly the divergences between both equations, even for large times, are actually very small, see figure 5.10. In some cases, while the steady state of (5.27) is not strictly thermal, the fidelity with that of (5.28) is more than 99.999%.

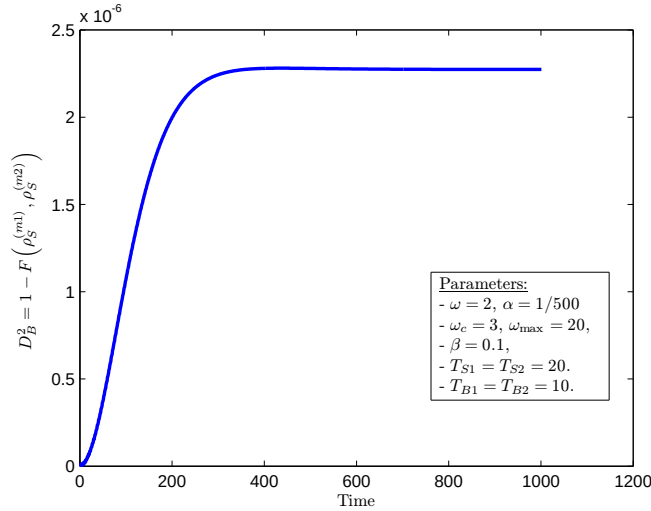


Figure 5.10: Fidelity between states $\rho_S^{(m1)}$ and $\rho_S^{(m2)}$ corresponding to master equations (5.27) and (5.28) respectively.

5.4 Driven Damped Harmonic Oscillator

One situation which is also interesting to analyze is that of adding a driving term in the Hamiltonian of the damped oscillator. At this stage we consider again

one single oscillator, damped by a thermal bath and driven by a coherent field (figure 5.11). This is described by a semiclassical Hamiltonian in the rotating wave approximation:

$$H(t) = \Omega a^\dagger a + r(a^\dagger e^{-i\omega^L t} + a e^{i\omega^L t}) + \sum_{j=1}^M \omega_j a_j^\dagger a_j + \sum_{j=1}^M g_j(a^\dagger a_j + a a_j^\dagger), \quad (5.33)$$

here ω^L is the frequency of the incident field and r the Rabi frequency.

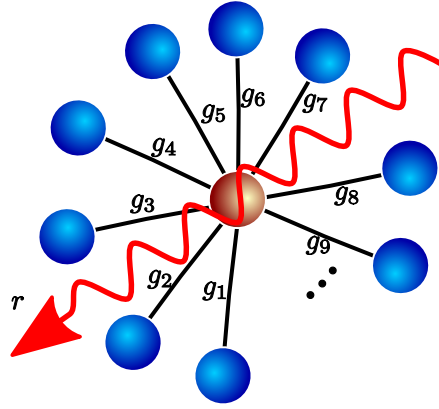


Figure 5.11: A single damped oscillator interacting with a classical incident field with Rabi frequency r .

5.4.1 Exact Solution

To obtain the exact solution of this system let us consider for a moment the Schrödinger picture,

$$\frac{d|\psi(t)\rangle}{dt} = -iH(t)|\psi(t)\rangle.$$

We solve this equation by means of the unitary transformation $U_{\text{rot}}(t) = e^{iH_{\text{rot}}t}$ where $H_{\text{rot}} = \omega^L (a^\dagger a + \sum_{j=1}^M a_j^\dagger a_j)$. Making the substitution $|\tilde{\psi}(t)\rangle = U_{\text{rot}}(t)|\psi(t)\rangle$ we immediately obtain

$$\frac{d|\tilde{\psi}(t)\rangle}{dt} = i[H_{\text{rot}} - U_{\text{rot}}(t)H(t)U_{\text{rot}}^\dagger(t)]|\tilde{\psi}(t)\rangle = -iH_0|\tilde{\psi}(t)\rangle,$$

where $H_0 = (\Omega - \omega^L)a^\dagger a + r(a + a^\dagger) + \sum_{j=1}^M (\omega_j - \omega^L)a_j^\dagger a_j + \sum_{j=1}^M g_j(a^\dagger a_j + a a_j^\dagger)$ is time-independent. Returning to the Schrödinger picture, the evolution of the states is then,

$$|\psi(t)\rangle = U(t, 0)|\psi(0)\rangle = e^{-iH_{\text{rot}}t}e^{-iH_0t}|\psi(0)\rangle.$$

In order to avoid differential equations with time-dependent coefficients, we can study the evolution in a X-P time rotating frame; in that frame the annihilation (and creation) operators $\tilde{a} = e^{-iH_{\text{rot}}t}ae^{iH_{\text{rot}}t}$ will evolve according to

$$\tilde{a}(t) = U^\dagger(t, 0)e^{-iH_{\text{rot}}t}ae^{iH_{\text{rot}}t}U(t, 0) = e^{iH_0t}ae^{-iH_0t}.$$

That is

$$i\dot{\tilde{a}} = [\tilde{a}, H_0] = (\Omega - \omega^L)\tilde{a} + \sum_{j=1}^M g_j\tilde{a}_j + r, \quad (5.34)$$

$$i\dot{\tilde{a}}_j = [\tilde{a}_j, H_0] = (\omega_j - \omega^L)\tilde{a}_j + g_j\tilde{a}, \quad (5.35)$$

which is quite similar to (5.12) but with the additional time-independent term r . Following the notation of section 5.2.2 we can write

$$i\dot{\tilde{A}} = W_0\tilde{A} + b,$$

here $b = (r, 0, \dots, 0)^T$ and W_0 is found from (5.15) as $W - \omega^L\mathbb{I}$. The solution of this system of differential equations is

$$\tilde{A}(t) = e^{-iW_0t} \left[A(0) - i \int_0^t ds e^{iW_0s} b \right].$$

If W_0 is invertible this equation can be written as

$$\tilde{A}(t) = e^{-iW_0t} [A(0) + W_0^{-1}b] - W_0^{-1}b, \quad (5.36)$$

Writing $T^0 = \exp -i w_0 t$, we can also compute the evolution of position and momentum operators $X = \frac{1}{\sqrt{2}}(A + A^\dagger)$ and $P = \frac{1}{\sqrt{2}i}(A - A^\dagger)$, as

$$\tilde{X}(t) = T_R^0 X(0) - T_I^0 P(0) + T_R^0 W_0^{-1} b - W_0^{-1} b, \quad (5.37)$$

$$\tilde{P}(t) = T_I^0 X(0) + T_R^0 P(0) + T_I^0 W_0^{-1} b, \quad (5.38)$$

where T_R^0 and T_I^0 are given by

$$T^0 = T_R + iT_I \Rightarrow \begin{cases} T_R^0 = \frac{T^0 + T^{0\dagger}}{2} = \cos(Wt) \\ T_I^0 = \frac{T^0 - T^{0\dagger}}{2i} = -\sin(Wt) \end{cases}. \quad (5.39)$$

Thus, by writing

$$\mathcal{M}^0 = \begin{pmatrix} T_R^0 & -T_I^0 \\ T_I^0 & T_R^0 \end{pmatrix}, \quad \mathcal{B} = \begin{pmatrix} (T_R^0 - \mathbb{I})W_0^{-1}b \\ T_I^0 W_0^{-1}b \end{pmatrix},$$

we find that the position and momentum expectation values evolve as

$$\tilde{R}(t) = \mathcal{M}^0 R(0) + \mathcal{B}. \quad (5.40)$$

Note that in this case the first moments of the state change, despite $\langle R(0) \rangle = 0$. To calculate the evolution of the covariance matrix, we proceed in the same way as before,

$$\begin{aligned} \langle \tilde{R}_i(t) \tilde{R}_j(t) \rangle &= \sum_{k,\ell} \mathcal{M}_{i,k}^0 \mathcal{M}_{j,\ell}^0 \langle R_i(0) R_j(0) \rangle + \sum_k \mathcal{M}_{i,k}^0 \langle R_k(0) \rangle \mathcal{B}_j \\ &\quad + \mathcal{B}_j \sum_k \mathcal{M}_{j,\ell}^0 \langle R_\ell(0) \rangle + \mathcal{B}_i \mathcal{B}_j. \end{aligned} \quad (5.41)$$

and analogously for the solutions for $\langle \tilde{R}_j(t) \tilde{R}_i(t) \rangle$ and $\langle \tilde{R}_i(t) \rangle \langle \tilde{R}_j(t) \rangle$. Combining these terms, we find the $\mathcal{B}$ cancel and so, in a similar fashion to (5.20), (5.20) and

(5.20),

$$\begin{aligned}\tilde{\mathcal{C}}_{1,1}(t) &= (\mathcal{M}_1^0, \mathcal{C}(0)\mathcal{M}_1^0), \\ \tilde{\mathcal{C}}_{1,M+2}(t) &= \tilde{\mathcal{C}}_{M+2,1}(t) = (\mathcal{M}_1^0, \mathcal{C}\mathcal{M}_{M+2}^0), \\ \tilde{\mathcal{C}}_{M+2,M+2}(t) &= (\mathcal{M}_{M+2}^0, \mathcal{C}\mathcal{M}_{M+2}^0),\end{aligned}\tag{5.42}$$

where, of course, $\mathcal{M}_1^0$ and $\mathcal{M}_2^0$ are as in (5.21) for $\mathcal{M}^0$.

5.4.2 Markovian Master Equations

In order to derive a master equation for this system we must take account of a couple of details. First, since the Hamiltonian is time-dependent the generator of the master equation must also be time-dependent,

$$\frac{d\rho_S(t)}{dt} = \mathcal{L}_t \rho_S(t),$$

whose solution defines a family of propagators $\mathcal{E}(t_2, t_1)$ such that

$$\begin{aligned}\rho_S(t_2) &= \mathcal{E}(t_2, t_1)\rho_S(t_1), \\ \mathcal{E}(t_3, t_1) &= \mathcal{E}(t_3, t_2)\mathcal{E}(t_2, t_1),\end{aligned}$$

These can be written formally as a time-ordered series

$$\mathcal{E}(t_1, t_0) = \mathcal{T} e^{\int_{t_0}^{t_1} \mathcal{L}_{t'} dt'},$$

where $\mathcal{T}$ is the well-known time-ordering operator. Similarly to the case of time-independent equations it can be shown that the family $\mathcal{E}(t_2, t_1)$ is completely positive for all $(t_2 \geq t_1)$ if and only if $\mathcal{L}_t$ has the Kossakowski-Lindblad form for any time t .

The second problem is that there is an absence of rigorous methods to arrive at a completely positive master equation in the Markovian limit when the Hamiltonian is time-dependent, with the exception of adiabatic regimes of ex-

ternal perturbations [99]. Fortunately in this case, due to the simple periodic time-dependence of the Hamiltonian, we will be able to obtain master equations valid for large (to some degree) Rabi frequencies, even though the complexity of the problem has increased. In our derivation, we will distinguish three cases: these will be when the Rabi frequency is very small; when the driving is far off resonance ($|\omega^L - \Omega| \gg 0$) and finally the identical case without the secular approximation.

The details of the derivation are left for Appendix 5.A.3, but in these three cases we find a Markovian master equation with the structure

$$\frac{d}{dt}\rho_S = -i[\bar{\Omega}a^\dagger a + \bar{r}e^{i\omega^L t}a + \bar{r}^*e^{-i\omega^L t}a^\dagger, \rho_S] + \mathcal{D}(\rho_S),$$

here $\mathcal{D}$ is given by (5.26), and $\bar{\Omega} = \Omega + \Delta$ is the same as for a single damped oscillator, and $\bar{r}$ is a renormalized Rabi frequency due to the effect of the bath. Note that as the incident field alters the position operator of the oscillator, which in turn couples to the bath, one should expect that the field is itself also effected by the environment. For small Rabi frequencies an argument similar to section 5.3.2 gives simply

$$\bar{r} = r, \tag{5.43}$$

whereas, when the driving field is far from resonance, $|\omega^L - \Omega| \gg 0$, we obtain

$$\bar{r} = r \left[1 + \frac{\Delta(\Omega) + i\gamma(\Omega)}{\Omega - \omega^L} \right]. \tag{5.44}$$

Finally, if we neglect the secular approximation, this regime yields

$$\bar{r} = r \left[1 + \frac{\Delta(\Omega) + i\gamma(\Omega)}{\Omega - \omega^L} - \frac{\Delta(\omega^L) + i\gamma(\omega^L)}{\Omega - \omega^L} \right]. \tag{5.45}$$

Without entering into the details of the derivation, one sees that equations (5.44) and (5.45) are problematic on resonance $|\Omega - \omega^L| \sim 0$. This is due to two approximations, one is the secular approximation in (5.44), and the other is the second order in the perturbative series. In the derivation in 5.A.3 it is clear why

in this case the series diverges for $|\Omega - \omega^L| \sim 0$.

5.4.3 Study of the Approximations

Note that in this case the range of validity of every equation is hazier than in previous sections, so which one is convenient is going to be discovered by the simulation, although one could suppose that the more elaborate equations (5.44) and (5.45) would provide the better approximation. However, there is still the question of how effective they are, and whether the additional effort required to obtain them is worthwhile in comparison to the simpler equation (5.43).

In addition note that in every case the covariance matrix is unaffected by the driving term, which only produce a change in the first moments. Furthermore, as the fidelity is invariant under unitary operations, we are always free to work in the frame rotating with the field. Therefore, all calculations can be performed with the rotating observables.

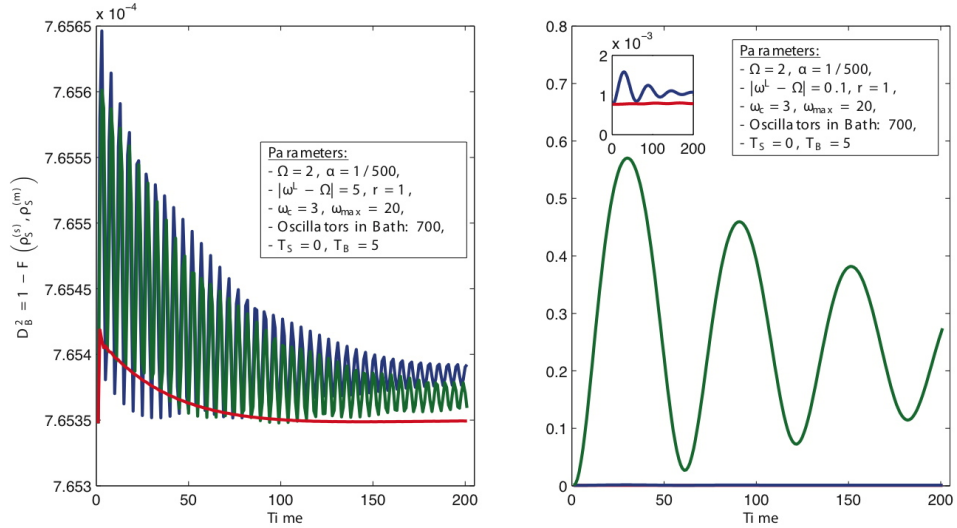


Figure 5.12: Fidelity between $\rho_S^{(s)}$ and $\rho_S^{(m)}$ for different renormalized Rabi frequencies (5.43) (blue), (5.44) (green) and (5.45) (red). An example of off resonance is shown on the left, whereas the plot on the right is close to resonance.

In figure 5.12 the fidelities are plotted for close to and far from resonance. Compare the amount of disagreement with the fidelity of a single damped oscil-

lator in figure 5.5. For global features, the more elaborate equation (5.45) works better in both cases, although the difference with (5.43) is very small. As expected, the choice of (5.44) is preferable over (5.43) when out of resonance, but gives quite poor results when close to resonance. However, when off resonance the difference among the three choices is essentially small.

Given these results, it is worthwhile to look at how the fidelities at one fixed time vary as a function of the detuning, this is done in figure 5.13.

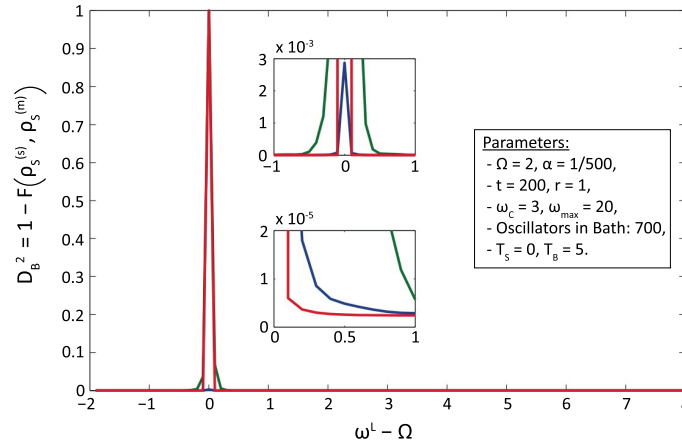


Figure 5.13: Fidelity between $\rho_S^{(s)}$ and $\rho_S^{(m)}$ for different renormalized Rabi frequencies (5.43) (blue), (5.44) (green) and (5.45) (red) as a function of the detuning.

Here we see that both (5.44) and (5.45) fail close to resonance, as was expected from the perturbative approach. Equation (5.43) gives good results due to the small Rabi frequency, however note in comparison to (5.45) the accuracy quickly drops off as we move away from $\omega^L - \Omega = 0$. A similar effect can be seen when compared to (5.44) for larger detunings.

Finally, in figure 5.14 we test the dependency of the fidelities on the strength of the Rabi frequencies far from resonance. Here the worst behaviour is observed for (5.43), as expected.

In summary, for the case of a driven damped harmonic oscillator the difference in accuracy among master equations is generally small. Equations (5.44) and (5.45) work better except in the case of resonance, where (5.43) gives more

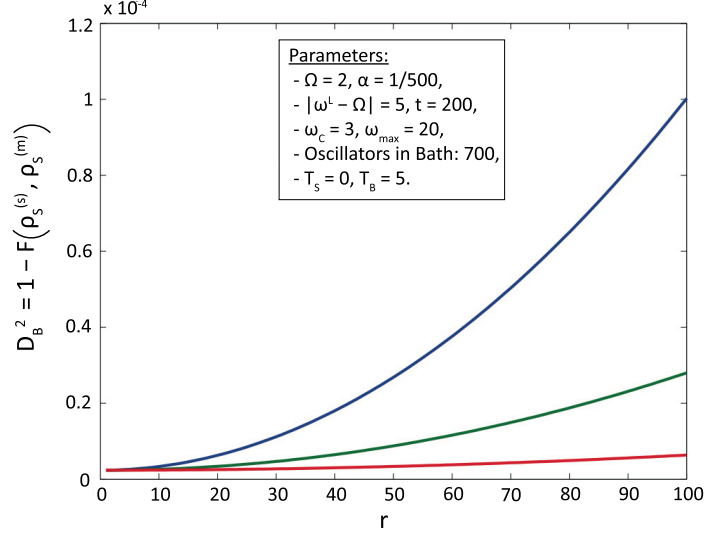


Figure 5.14: Fidelity between $\rho_S^{(s)}$ and $\rho_S^{(m)}$ for different renormalized Rabi frequencies (5.43) (blue), (5.44) (green) and (5.45) (red) as a function of the Rabi frequency.

accurate results, as long as the Rabi frequency is small. To use of one equation over another will depend on the context and the accuracy which one wants to obtain, but given that the differences are so small that the simplest choice (5.43) seems to be the more “economical” way to describe the dynamics.

5.5 Conclusions

In this chapter we have shown how one can derive a number of different Markovian master equations for harmonic oscillators and studied their range of validity by means of exactly simulating the dynamics of Gaussian systems. In particular,

- We have clarified the possible detrimental effect of low temperatures on the Markovian treatment of a damped oscillator, showing that the Markovian master equation provides good accuracy regardless of the temperature of the bath.
- We have shown that the system-environment state factorization assumption for all times has to be understood in general as an effective model by deriving

the same equation using the projection operator technique.

- We analysed two strategies for finding completely positive Markovian master equations for two harmonic oscillators coupled together under the effect of local baths, indicating that both are complementary in their range of validity. Moreover, when the temperature of the local baths is the same the difference between them is quite small.
- In the same spirit, we derived time inhomogeneous completely positive Markovian master equations for a damped oscillator which is driven by an external classical field. We studied the validity of each one and pointed out that completely positive dynamics can be obtained even without secular approximation (for these kinds of inhomogeneous equations).

Despite the fact that we have focused on harmonic oscillator systems, the proposed method is general and we expect that non-harmonic systems should behave in a similar manner with respect to the validity of the equations. This suggests that the general conclusions made here are widely applicable to any other settings involving a weak interaction with an environment.

In this regard, we hope that the present study may help in providing a better understanding and a transparent description of noise in interacting systems, including those situations where the strength of the internal system interaction is large. There are currently many quantum scenarios open to the use of these techniques, including realizations of harmonic and spin chains in systems of trapped ions [107], superconducting qubits [108] and nitrogen-vacancy (NV) defects in diamond.

Moreover, interacting systems subject to local reservoirs have been recently treated under the assumption of weak internal system interaction in theoretical studies ranging from the excitation transport properties of biomolecules to the stability of topological codes for quantum information [100].

5.A Derivation of Master equations

5.A.1 Two coupled damped harmonic oscillators, small β

We can derive Markovian Master equations like (5.27) from the microscopic model by the following procedure. The Von Neumann equation in the interaction picture with respect to the free Hamiltonian $H_{\text{free}} = H_{01} + H_{02} + H_{B1} + H_{B2}$ is

$$\begin{aligned} \frac{d}{dt}\tilde{\rho}(t) &= -i\beta[\tilde{V}_{12}(t), \tilde{\rho}(t)] - i\alpha[\tilde{V}_{SB}(t), \tilde{\rho}(t)] \\ &\equiv \beta\mathcal{V}_{12}(t)\tilde{\rho}(t) + \alpha\mathcal{V}_{SB}(t)\tilde{\rho}(t), \end{aligned} \quad (5.46)$$

where $\tilde{V}_{SB}(t) = \tilde{V}_{1B1}(t) + \tilde{V}_{2B2}(t)$ and for simplicity we have assumed that the strength of the coupling with each bath is identical (the reader will note afterwards that this is not a crucial assumption). We now define the projector $\mathcal{P}\rho(t) = \text{Tr}_{(B1, B2)}[\rho(t)] \otimes \rho_{\text{th}1} \otimes \rho_{\text{th}2}$, along with $\mathcal{Q} = \mathbb{I} - \mathcal{P}$. The application of the projection operators on (5.46) yields

$$\frac{d}{dt}\mathcal{P}\tilde{\rho}(t) = \beta\mathcal{P}\mathcal{V}_{12}(t)\tilde{\rho}(t) + \alpha\mathcal{P}\mathcal{V}_{SB}(t)\tilde{\rho}(t), \quad (5.47)$$

$$\frac{d}{dt}\mathcal{Q}\tilde{\rho}(t) = \beta\mathcal{Q}\mathcal{V}_{12}(t)\tilde{\rho}(t) + \alpha\mathcal{Q}\mathcal{V}_{SB}(t)\tilde{\rho}(t), \quad (5.48)$$

and so (c.f. section 4.1.1) we find a formal solution to the second equation as

$$\begin{aligned} \mathcal{Q}\tilde{\rho}(t) &= \mathcal{G}(t, t_0)\mathcal{Q}\tilde{\rho}(t_0) + \beta \int_{t_0}^t ds \mathcal{G}(t, s)\mathcal{Q}\mathcal{V}_{12}(s)\mathcal{P}\tilde{\rho}(s) \\ &\quad + \alpha \int_{t_0}^t ds \mathcal{G}(t, s)\mathcal{Q}\mathcal{V}_{SB}(s)\mathcal{P}\tilde{\rho}(s), \end{aligned} \quad (5.49)$$

where

$$\mathcal{G}(t, s) = \mathcal{T}e^{\int_s^t dt' [\beta\mathcal{V}_{12}(t') + \alpha\mathcal{V}_{SB}(t')]}.$$

Now the procedure is as follows, we introduce the identity $\mathbb{I} = \mathcal{P} + \mathcal{Q}$ in the second term of equation (5.47),

$$\frac{d}{dt}\mathcal{P}\tilde{\rho}(t) = \beta\mathcal{P}\mathcal{V}_{12}(t)\tilde{\rho}(t) + \alpha\mathcal{P}\mathcal{V}_{SB}(t)\mathcal{P}\tilde{\rho}(t) + \alpha\mathcal{P}\mathcal{V}_{SB}(t)\mathcal{Q}\tilde{\rho}(t),$$

and insert the formal solution (5.49) into the last term. Recalling the condition (4.2) $\mathcal{P}\mathcal{V}\mathcal{P} = 0$ and again assuming an initial factorised state ($\mathcal{Q}\rho(t_0) = 0$) we find

$$\frac{d}{dt}\mathcal{P}\tilde{\rho}(t) = \beta\mathcal{P}\mathcal{V}_{12}(t)\tilde{\rho}(t) + \int_{t_0}^t ds\mathcal{K}_1(t,s)\mathcal{P}\tilde{\rho}(s) + \int_{t_0}^t ds\mathcal{K}_2(t,s)\mathcal{P}\tilde{\rho}(s),$$

where here the kernels are

$$\begin{aligned}\mathcal{K}_1(t,s) &= \alpha\beta\mathcal{P}\mathcal{V}_{SB}(t)\mathcal{G}(t,s)\mathcal{Q}\mathcal{V}_{12}(s)\mathcal{P} = 0, \\ \mathcal{K}_2(t,s) &= \alpha^2\mathcal{P}\mathcal{V}_{SB}(t)\mathcal{G}(t,s)\mathcal{Q}\mathcal{V}_{SB}(s)\mathcal{P}.\end{aligned}$$

The first vanishes because $\mathcal{V}_{12}(s)$ commutes with $\mathcal{P}$ and $\mathcal{Q}\mathcal{P} = 0$. If we consider the second kernel, weak coupling implies $\alpha \gtrsim \beta$, and so to second order in α and β this becomes

$$\mathcal{K}_2(t,s) = \alpha^2\mathcal{P}\mathcal{V}_{SB}(t)\mathcal{Q}\mathcal{V}_{SB}(s)\mathcal{P} + \mathcal{O}(\alpha^3, \alpha^2\beta),$$

which has exactly the same form as (4.6) and therefore the equation of motion becomes

$$\frac{d}{dt}\mathcal{P}\tilde{\rho}(t) = \beta\mathcal{P}\mathcal{V}_{12}(t)\tilde{\rho}(t) + \alpha^2 \int_{t_0}^t ds\mathcal{P}\mathcal{V}_{SB}(t)\mathcal{V}_{SB}(s)\mathcal{P}\tilde{\rho}(s).$$

Finally we note that

$$\text{Tr}_{B1,B2} \left[\tilde{V}_{1B1}(t)\tilde{V}_{2B2}(t') (\rho_{\text{th}1} \otimes \rho_{\text{th}2}) \right] = \text{Tr}_{B1}[\tilde{V}_{1B1}(t)\rho_{\text{th}1}] \text{Tr}_{B2}[\tilde{V}_{2B2}(t')\rho_{\text{th}2}] = 0,$$

because our interactions individually hold $\text{Tr}_{B1}[\tilde{V}_{1B1}\rho_{\text{th}1}] = \text{Tr}_{B2}[\tilde{V}_{2B2}\rho_{\text{th}2}] = 0$, so $\mathcal{P}\mathcal{V}_{1B1}\mathcal{V}_{2B2}\mathcal{P} = \mathcal{P}\mathcal{V}_{2B2}\mathcal{V}_{1B1}\mathcal{P} = 0$ and then

$$\begin{aligned}\frac{d}{dt}\mathcal{P}\tilde{\rho}(t) &= \beta\mathcal{P}\mathcal{V}_{12}(t)\tilde{\rho}(t) + \alpha^2 \int_{t_0}^t ds\mathcal{P}\mathcal{V}_{1B1}(t)\mathcal{V}_{1B1}(s)\mathcal{P}\tilde{\rho}(s) \\ &\quad + \alpha^2 \int_{t_0}^t ds\mathcal{P}\mathcal{V}_{2B2}(t)\mathcal{V}_{2B2}(s)\mathcal{P}\tilde{\rho}(s),\end{aligned}$$

which may be rewritten as

$$\begin{aligned} \frac{d}{dt}\tilde{\rho}_S(t) = & -i\beta[\tilde{V}_{12}(t), \tilde{\rho}_S(t)] - \beta \int_{t_0}^t dt' \text{Tr}_{B1}[\tilde{V}_{1B1}(t), [\tilde{V}_{1B1}(t'), [\tilde{\rho}_S(t') \otimes \tilde{\rho}_{\text{th1}}(t')]]] \\ & - \beta \int_{t_0}^t dt' \text{Tr}_{B2}[\tilde{V}_{2B2}(t), [\tilde{V}_{2B2}(t'), [\tilde{\rho}_S(t') \otimes \tilde{\rho}_{\text{th2}}(t')]]]. \end{aligned} \quad (5.50)$$

The last quantity of the above equation is just a sum of the individual terms for each bath, which lead, under the standard procedure of section 4.1.1, to the (interaction picture) local dissipators $\mathcal{D}_1$ and $\mathcal{D}_2$ and shifts of (5.27).

5.A.2 Two coupled damped harmonic oscillators, large β

First, let us write the Hamiltonian of the two oscillator system in a more convenient way

$$H_{12} = H_{01} + H_{02} + V_{12} = (a_1^\dagger, a_2^\dagger) \begin{pmatrix} \Omega_1 & \beta \\ \beta & \Omega_2 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \end{pmatrix}.$$

We can diagonalize this quadratic form by means of a rotation to get

$$H_{12} = \Omega_+ b_1^\dagger b_1 + \Omega_- b_2^\dagger b_2,$$

where

$$\Omega_\pm = \frac{(\Omega_1 + \Omega_2) \pm \sqrt{4\beta^2 + (\Omega_1 - \Omega_2)^2}}{2},$$

and the creation and annihilation operators in the rotated frame are given by

$$\begin{aligned} b_1 &= a_1 \cos(\alpha) - a_2 \sin(\alpha), \\ b_2 &= a_1 \sin(\alpha) + a_2 \cos(\alpha), \end{aligned}$$

with the angle specified by

$$\tan(\alpha) = \frac{2\beta}{(\Omega_1 - \Omega_2) - \sqrt{4\beta^2 + (\Omega_1 - \Omega_2)^2}}.$$

The new operators satisfy the standard bosonic commutation rules $[b_i, b_j^\dagger] = \delta_{ij}$, and so this is nothing more than the decomposition of an oscillatory system in normal modes. For simplicity, let us now take $\Omega_1 = \Omega_2 = \Omega$, and so

$$\Omega_{\pm} = \Omega \pm \beta, \quad \begin{cases} b_1 = \frac{1}{\sqrt{2}}(a_1 + a_2) \\ b_2 = \frac{1}{\sqrt{2}}(a_1 - a_2) \end{cases},$$

note that RWA approximation implies $\Omega \gg \beta$ so both normal mode frequencies are positive.

We can reexpress the interactions with the baths in terms of these new operators,

$$\begin{aligned} V_{1B1} &= \sum_{j=1}^M \frac{g_{1j}}{\sqrt{2}} [(b_1^\dagger + b_2^\dagger)a_{1j} + (b_1 + b_2)a_{1j}^\dagger], \\ V_{2B2} &= \sum_{j=1}^M \frac{g_{2j}}{\sqrt{2}} [(b_1^\dagger - b_2^\dagger)a_{2j} + (b_1 - b_2)a_{2j}^\dagger], \end{aligned}$$

the benefit of this is that it allows us to easily deal with the interaction picture with respect to $H_0 = H_{12} + H_{B1} + H_{B2}$. By following the method of section 4.1.1 we obtain the analog of (4.8),

$$\begin{aligned} \frac{d}{dt} \tilde{\rho}_S(t) &= - \int_0^\infty dt' \text{Tr}_{B1} [\tilde{V}_{1B1}(t), [\tilde{V}_{1B1}(t-s), \tilde{\rho}_S(t) \otimes \rho_{\text{th1}}]] \\ &\quad - \int_0^\infty ds \text{Tr}_{B2} [\tilde{V}_{2B2}(t), [\tilde{V}_{2B2}(t-s), \tilde{\rho}_S(t) \otimes \rho_{\text{th2}}]]. \end{aligned} \quad (5.51)$$

where we have noted $\mathcal{P}\mathcal{V}_{1B1}\mathcal{V}_{2B2}\mathcal{P} = \mathcal{P}\mathcal{V}_{2B2}\mathcal{V}_{1B1}\mathcal{P} = 0$. Each of the above terms correspond, essentially, to one of a pair of two free harmonic oscillators with frequencies Ω_+ and Ω_- , coupled to a common bath. Consequently, we can deal

with them separately. Starting with the first term

$$\mathcal{L}_1(\tilde{\rho}_S) = - \int_0^t ds \operatorname{Tr}_{B1}[\tilde{V}_{1B1}(t), [\tilde{V}_{1B1}(t-s), \tilde{\rho}_S(t-s) \otimes \rho_{\text{th}1}]], \quad (5.52)$$

we decompose the interaction in to eigenoperators of $[H_{12}, \cdot]$ (see (4.11))

$$V_{1B1} = \sum_k A_k \otimes B_k, \quad (5.53)$$

with

$$\begin{aligned} A_1 &= \frac{1}{\sqrt{2}}(b_1 + b_2), & A_2 &= \frac{1}{\sqrt{2}}(b_1^\dagger + b_2^\dagger), \\ B_1 &= \sum_{j=1}^M g_{1j} a_{1j}^\dagger, & B_2 &= \sum_{j=1}^M g_{1j} a_{1j}, \end{aligned} \quad (5.54)$$

Notice the A_1 operator can be written as $A_1 = A_1(\Omega_+) + A_1(\Omega_-)$, where $A_1(\Omega_+) = b_1/\sqrt{2}$ and $A_1(\Omega_-) = b_2/\sqrt{2}$ are already the eigenoperators of $[H_{12}, \cdot]$ with eigenvalues $-\Omega_+$ and $-\Omega_-$ respectively. Similarly $A_2 = A_2(-\Omega_+) + A_2(-\Omega_-)$, with $A_2(-\Omega_+) = b_1^\dagger/\sqrt{2}$ and $A_2(-\Omega_-) = b_2^\dagger/\sqrt{2}$, and so we can write (5.53) as

$$V_{1B1} = \sum_k A_k \otimes B_k = \sum_{\nu, k} A_k(\nu) \otimes B_k = \sum_{\nu, k} A_k^\dagger(\nu) \otimes B_k^\dagger, \quad (5.55)$$

which in the interaction picture becomes

$$\tilde{V}_{1B1}(t) = \sum_{\nu, k} e^{-i\nu t} A_k(\nu) \otimes \tilde{B}_k(t) = \sum_{\nu, k} e^{i\nu t} A_k^\dagger(\nu) \otimes \tilde{B}_k^\dagger(t).$$

Now, for the first element of (4.13) we have

$$\begin{aligned} \Gamma_{1,1}(\nu) &= \sum_{j, j'} g_{1j} g_{1j'} \int_0^\infty ds e^{i(\nu - \omega_{1j})s} \operatorname{Tr} \left(\rho_{B1}^{\text{th}} a_{1j} a_{1j'}^\dagger \right) \\ &= \sum_{j=1}^M g_{1j}^2 \int_0^\infty ds e^{i(\nu - \omega_{1j})s} [\bar{n}_1(\omega_{1j}) + 1], \end{aligned} \quad (5.56)$$

where the mean number of quanta in the first bath with frequency ω_{1j} , $\bar{n}_1(\omega_{1j})$, is given by the Bose-Einstein distribution (5.5). Going to the continuous limit we take $M \rightarrow \infty$ and introduce the spectral density of the first bath $J_1(\omega) = \sum_j g_{1j}^2 \delta(\omega - \omega_{1j})$,

$$\Gamma_{1,1}(\nu) = \int_0^\infty d\omega J_1(\omega) \int_0^\infty ds e^{i(\nu-\omega)s} [\bar{n}_1(\omega) + 1].$$

Now using the well-know formula from distribution theory,

$$\int_0^\infty dx e^{ixy} = \pi \delta(y) + i \text{P.V.} \left(\frac{1}{y} \right),$$

and assuming $\nu > 0$, we split into real and imaginary parts,

$$\Gamma_{1,1}(\nu) = \gamma_1(\nu) [\bar{n}_1(\nu) + 1] + i [\Delta_1(\nu) + \Delta'_1(\nu)],$$

where

$$\begin{aligned} \gamma_1(\nu) &= \pi J_1(\nu), \\ \Delta_1(\nu) &= \text{P.V.} \int_0^\infty d\omega \frac{J_1(\omega)}{\nu - \omega}, \\ \Delta'_1(\nu) &= \text{P.V.} \int_0^\infty d\omega \frac{J_1(\omega) \bar{n}_1(\omega)}{\nu - \omega}. \end{aligned} \tag{5.57}$$

Similar calculations give ($\nu > 0$)

$$\Gamma_{1,2}(-\nu) = \Gamma_{2,1}(\nu) = 0, \tag{5.58}$$

$$\Gamma_{2,2}(-\nu) = \gamma_1(\nu) \bar{n}_1(\nu) - i \Delta'_1(\nu). \tag{5.59}$$

Thus, equation (5.52) becomes

$$\begin{aligned}
\mathcal{L}_1(\tilde{\rho}_S) = & \sum_{\nu, \nu'} e^{i(\nu' - \nu)t} \Gamma_{1,1}(\nu) [A_1(\nu) \tilde{\rho}_S(t), A_1^\dagger(\nu')] \\
& + e^{i(\nu - \nu')t} \Gamma_{1,1}^*(\nu) [A_1(\nu'), \tilde{\rho}_S(t) A_1^\dagger(\nu)] \\
& + e^{i(\nu' - \nu)t} \Gamma_{2,2}(\nu) [A_2(\nu) \tilde{\rho}_S(t), A_2^\dagger(\nu')] \\
& + e^{i(\nu - \nu')t} \Gamma_{2,2}^*(\nu) [A_2(\nu'), \tilde{\rho}_S(t) A_2^\dagger(\nu)]. \tag{5.60}
\end{aligned}$$

Now we perform the secular approximation; the cross terms $\nu' \neq \nu$ in the above expression, which go as $e^{\pm 2\beta t i}$, can be neglected provided that 2β is large in comparison with the inverse of the relaxation rate ($\beta \gg \alpha$) and so we obtain

$$\begin{aligned}
\mathcal{L}_1(\tilde{\rho}_S) = & -i \frac{\Delta_1(\Omega_+)}{2} [b_1^\dagger b_1, \tilde{\rho}_S(t)] - i \frac{\Delta_1(\Omega_-)}{2} [b_2^\dagger b_2, \tilde{\rho}_S(t)] \\
& + \gamma_1(\Omega_+) [\bar{n}_1(\Omega_+) + 1] \left(b_1 \tilde{\rho}_S(t) b_1^\dagger - \frac{1}{2} \{b_1^\dagger b_1, \tilde{\rho}_S(t)\} \right) \\
& + \gamma_1(\Omega_+) \bar{n}_1(\Omega_+) \left(b_1^\dagger \tilde{\rho}_S(t) b_1 - \frac{1}{2} \{b_1 b_1^\dagger, \tilde{\rho}_S(t)\} \right) \\
& + \gamma_1(\Omega_-) [\bar{n}_1(\Omega_-) + 1] \left(b_2 \tilde{\rho}_S(t) b_2^\dagger - \frac{1}{2} \{b_2^\dagger b_2, \tilde{\rho}_S(t)\} \right) \\
& + \gamma_1(\Omega_-) \bar{n}_1(\Omega_-) \left(b_2^\dagger \tilde{\rho}_S(t) b_2 - \frac{1}{2} \{b_2 b_2^\dagger, \tilde{\rho}_S(t)\} \right).
\end{aligned}$$

Returning to equation (5.51), for the second term,

$$\mathcal{L}_2(\tilde{\rho}_S) = - \int_0^\infty ds \operatorname{Tr}_{B1} [\tilde{V}_{2B2}(t), [\tilde{V}_{2B2}(t-s), \tilde{\rho}_S(t) \otimes \rho_{\text{th}2}]],$$

the situation is essentially the same, since the minus sign in b_2 only modifies the cross terms, which we neglect in the secular approximation. Following similar steps as in the above we obtain the same form (5.61) for $\mathcal{L}_2$, with the replacements $\gamma_1 \rightarrow \gamma_2$, $\Delta_1 \rightarrow \Delta_2$ and $\bar{n}_1 \rightarrow \bar{n}_2$, where the subscript 2 refers to the corresponding expression with the spectral density and temperature of the second bath. There-

fore putting together both quantities, and returning to the Schrödinger picture

$$\begin{aligned}
\frac{d}{dt}\rho_S(t) = & -i [\Omega_1 + \Delta_1(\Omega_+)/2 + \Delta_2(\Omega_+)/2] [b_1^\dagger b_1, \rho_S(t)] \\
& -i [\Omega_2 + \Delta_1(\Omega_-)/2 + \Delta_2(\Omega_-)/2] [b_2^\dagger b_2, \rho_S(t)] \\
& + \{\gamma_1(\Omega_+)[\bar{n}_1(\Omega_+) + 1] + \gamma_2(\Omega_+)[\bar{n}_2(\Omega_+) + 1]\} \left(b_1 \rho_S(t) b_1^\dagger - \frac{1}{2} \{b_1^\dagger b_1, \rho_S(t)\} \right) \\
& + [\gamma_1(\Omega_+) \bar{n}_1(\Omega_+) + \gamma_2(\Omega_+) \bar{n}_2(\Omega_+)] \left(b_1^\dagger \rho_S(t) b_1 - \frac{1}{2} \{b_1 b_1^\dagger, \rho_S(t)\} \right) \\
& + \{\gamma_1(\Omega_-)[\bar{n}_1(\Omega_-) + 1] + \gamma_2(\Omega_-)[\bar{n}_2(\Omega_-) + 1]\} \left(b_2 \rho_S(t) b_2^\dagger - \frac{1}{2} \{b_2^\dagger b_2, \rho_S(t)\} \right) \\
& + [\gamma_1(\Omega_-) \bar{n}_1(\Omega_-) + \gamma_2(\Omega_-) \bar{n}_2(\Omega_-)] \left(b_2^\dagger \rho_S(t) b_2 - \frac{1}{2} \{b_2 b_2^\dagger, \rho_S(t)\} \right).
\end{aligned} \tag{5.61}$$

It is manifestly clear that this equation is of the Kossakowski-Lindblad form. Finally, we rewrite the operators b_1 and b_2 in terms of a_1 and a_2 to arrive at equation (5.28).

It is worth mentioning that similar equations for coupled harmonic oscillators have been given previously (see for example [101, 102]), but not in the Kossakowski-Lindblad form, since in those derivations the secular approximation is not taken.

5.A.3 Driven damped harmonic oscillator

To derive a completely positive master equation valid for large Rabi frequencies r we must work in the interaction picture generated by the unitary propagator $U(t_1, t_0) = \mathcal{T} e^{-i \int_{t_0}^{t_1} H_1(t') dt'}$, where

$$H_1(t) = \Omega a^\dagger a + r(a^\dagger e^{-i\omega^L t} + a e^{i\omega^L t}) + \sum_{j=1}^M \omega_j a_j^\dagger a_j. \tag{5.62}$$

Taking $t_0 = 0$ without loss of generality, the time-evolution equation for $\tilde{\rho}(t) = U^\dagger(t, 0)\rho(t)U(t, 0)$ is

$$\dot{\tilde{\rho}}(t) = -i[\tilde{V}(t), \tilde{\rho}(t)], \tag{5.63}$$

so by following the analogous procedure for time-independent generators, one immediately deals with the problem that is not clear whether there exist something similar to the eigenoperator decomposition of $\tilde{V}(t) = U^\dagger(t, 0)VU(t, 0)$ ($V = \sum_{j=1}^M g_j(a^\dagger a_j + a a_j^\dagger)$) as in (4.10) and (4.11). Note however that the operator $\tilde{A}_1(t) = \tilde{a}(t)$ satisfies a differential equation with periodic terms

$$i\dot{\tilde{a}}(t) = [\tilde{a}(t), H_0(t)] = \Omega\tilde{a}(t) + r e^{-i\omega^L t}. \quad (5.64)$$

This kind of equation can be studied with the well-established Floquet theory (see for example [81, 82]), particularly it is possible to predict if its solution is a periodic function. In such a case, the operator in the new picture would have a formal decomposition similar to that in (4.10) and (4.11), such that $\tilde{A}_k(t) = \sum_\nu A_k(\nu) e^{i\nu t}$. This would then allow us to follow a similar procedure to that for time-independent Hamiltonians. Note that the importance of such a decomposition is that the operators $A_k(\nu)$ are themselves time-independent. Such ideas have already been used before in, for instance, [103, 104].

The solution to equation (5.64), with the initial condition $\tilde{a}(0) = a$ and for $\Omega \neq \omega^L$ is given by

$$\tilde{a}(t) = \frac{r(e^{-i\omega^L t} - e^{-i\Omega t}) + a(\omega^L - \Omega)e^{-i\Omega t}}{\omega^L - \Omega}, \quad (5.65)$$

so in this case the solution is periodic and the desired decomposition $\tilde{A}_1(t) = \sum_\nu A_1(\nu) e^{i\nu t}$ is

$$\tilde{A}_1(t) = A_1(\omega^L) e^{-i\omega^L t} + A_2(\Omega) e^{-i\Omega t},$$

where $A_1(\omega^L) = \frac{r}{\omega^L - \Omega} \mathbb{I}$ and $A_1(\Omega) = a - \frac{r}{\omega^L - \Omega} \mathbb{I} = a - A_1(\omega^L)$. Similarly

$$\tilde{A}_2(t) = A_2(-\omega^L) e^{i\omega^L t} + A_2(-\Omega) e^{i\Omega t},$$

with $A_2(-\omega^L) = \frac{r}{\omega^L - \Omega} \mathbb{I} = A_1(\omega^L)$ and $A_2(-\Omega) = a^\dagger - \frac{r}{\omega^L - \Omega} \mathbb{I} = a - A_2(-\omega^L)$.

Thus we get an equation analogous to (5.60), where the coefficients are:

$$\begin{aligned}\Gamma_{11}(\nu) &= \gamma(\nu)[\bar{n}(\nu) + 1] + i[\Delta(\nu) + \Delta'(\nu)], \quad (\nu > 0) \\ \Gamma_{12}(\nu) &= \Gamma_{21}(\nu) = 0, \\ \Gamma_{22}(\nu) &= \gamma(-\nu)\bar{n}(-\nu) - i\Delta'(-\nu) \quad (\nu < 0).\end{aligned}$$

Before continuing note that in the perturbative series of (5.63), the “strength” of the interaction $\tilde{V}(t)$ is now not solely dependent on the coupling with the bath. This is because the operators $A(\nu)$ depend linearly on $\frac{r}{w^L - \Omega}$, so when this ratio becomes large we expect that the approximation breaks down, i.e. for $r \gg 1$ or very close to resonance $|w^L - \Omega| \approx 0$.

Next we assume that the detuning is large enough $|\omega^L - \Omega| \gg \alpha$, $|\omega^L - \Omega|^2 \gg \alpha r$ in order to make the secular approximation and after some tedious, but straightforward, algebra we find the master equation in the interaction picture to be

$$\begin{aligned}\frac{d}{dt}\tilde{\rho}_S &= -i[\Delta(\Omega)a^\dagger a - \frac{\Delta(\Omega)r}{\omega^L - \Omega}(a + a^\dagger) \\ &\quad + \frac{\gamma(\Omega)r}{\omega^L - \Omega} \frac{a - a^\dagger}{i}, \tilde{\rho}_S] + \mathcal{D}(\tilde{\rho}_S),\end{aligned}\tag{5.66}$$

where $\mathcal{D}(\cdot)$ has again the form of (5.26). Finally, on returning to the Schrödinger picture we have,

$$\begin{aligned}\frac{d}{dt}\rho_S &= -i[H_1(t), \rho_S] + U(t, 0)\dot{\rho}_S U^\dagger(t, 0) \\ &= -i[\bar{\Omega}a^\dagger a + \bar{r}e^{i\omega^L t}a + \bar{r}^*e^{-i\omega^L t}a^\dagger, \rho_S] + D(\rho_S),\end{aligned}\tag{5.67}$$

where $\bar{\Omega} = \Omega + \Delta(\Omega)$ and

$$\bar{r} = r \left[1 + \frac{\Delta(\Omega) + i\gamma(\Omega)}{\Omega - \omega^L} \right].\tag{5.68}$$

So in this master equation the Rabi frequency is renormalized by the effect of the bath. It is worth noting, that even though in this master equation the Rabi

frequency is renormalised by the effect of the bath, at first order in r and the coupling α we obtain equation (5.25). This is as expected, given the arguments in section 5.3.2.

For an arbitrary driving frequency a Markovian master equation is difficult to obtain as we cannot, in general, make the secular approximation (apart from the perturbative condition $|w^L - \Omega| \approx 0$). This can be illustrated in the extreme case of resonance $\omega^L = \Omega$. Solving equation (5.64) under this condition we find

$$\tilde{a}(t) = e^{-i\Omega t}(a - irt), \quad (5.69)$$

and so one can see that $\tilde{a}(t)$ is not a periodic function, so the desired decomposition as a sum of exponentials with time-independent coefficients does not exist. On the other hand, the decomposition (5.65) tends to (5.69) in the limit $\omega^L \rightarrow \Omega$, so we may attempt to work with this decomposition and wonder whether on resonance the new master equation holds in this limit as well (in fact, we have shown that this is not true in section 5.4.3). The only problem to deal with is the possible lack of positivity due to the absence of the secular approximation. However, note that in this particular case only a commutator term arises from the cross terms in the analog of equation (5.60), so positivity is not lost. In fact, we obtain an equation similar to (5.67) except for an additional correction to the Rabi frequency:

$$\bar{r} = r \left[1 + \frac{\Delta(\Omega) + i\gamma(\Omega)}{\Omega - \omega^L} - \frac{\Delta(\omega^L) + i\gamma(\omega^L)}{\Omega - \omega^L} \right]. \quad (5.70)$$

Note that to first order in r and α we again obtain the equation (5.25).

Chapter 6

Smooth Entropies in Continuous Variables

6.1 Introduction

In many operational interpretations of the Shannon/von Neumann entropy there is typically an underlying assumption that quantities are defined asymptotically and under the condition that processes are repeated a large number of times. That is, we expect the random variables or probability distributions to be independent and identically distributed (i.i.d). For example, one may be interested in the rate at which data can be transmitted reliably through a communication channel (channel capacity), or in the amount of space needed to store a signal perfectly (compression) [52]. In each case, these operational quantities are defined based on a large number of mutually independent usages, be it either in the number of pieces of data or uses of a channel. The relevant entropy measure is then either the Shannon entropy, if the system is classical, or the von Neumann entropy if it is quantum.

In some situations, however, we cannot rely on the i.i.d assumption, and instead require a set of measures more suited to “single shot” scenarios. These can be provided by the (*smooth*) *min- and max- entropies* [53], which in the uncondi-

tional versions emerge as the limiting quantities in a family of measures known as the Rényi entropies (see Sec 6.3). The measures admit a number of operational interpretations. For the smooth max-entropy, $H_{\max}^\epsilon(X)$, we can ask the question, what is the minimum length, $l_{\text{compr}}^\epsilon(X)$ of an encoding from which the value of a single realisation of a random variable can be recovered with probability $1 - \epsilon$? The answer to this is given by [53],

$$l_{\text{compr}}^\epsilon(X) = H_{\max}^{\epsilon'}(X) + O(\log 1/\epsilon), \quad (6.1)$$

with $\epsilon \in [\frac{1}{2}\epsilon, 2\epsilon]$.

On the other hand, the min-entropy plays a crucial role in *randomness extraction*. From the leftover hash lemma, $H_{\min}(X)$ gives the maximum number of independent uniformly random bits which can be extracted from a given random variable.

The purpose of this chapter is to explore the relevance of these measures to the thermodynamic setting. In particular, we shall ask the question, what is the most appropriate entropy measure for describing the process of thermalisation? A particular example of this would be in the equilibration of small quantum systems. Where here the usual thermodynamic entropy for large, uncorrelated systems may no longer make sense. Instead we shall consider the role of the min-entropy and provide evidence that this may stabilise on timescales slower than the von Neumann entropy.

There is however a caveat. For very small subsystems, such as those we can hope to model exactly (say with qubits, for example), perturbations from the boundaries mean observing a true equilibration is often impossible. In order to overcome this problem, we are forced to consider subsystems large enough that these effects don't play too great a role. However, modeling such systems is in general computationally very taxing [55], especially if one tries to include the environment in a realistic manner. Instead, we shall tackle the problem using Gaussian states, for which both large systems, and approximate environment models are feasible. The first step is then developing suitable methods of evaluating the

smooth min- (and max-) entropies for Gaussian states. As our starting point, we shall take the covariance matrix, providing expressions relating the symplectic eigenvalues to each measure. These will then allow us to study the dynamics of equilibrating thermodynamic systems for which deviation in the entropies can be expected.

This chapter is organised as follows. First we shall explicitly state our notion of thermalisation. For this we shall adopt the approach of Popescu *et al.* [11, 54]. We will then introduce the min- and max- entropies, and show how smooth versions can be defined. In Section 6.4 we will then derive expressions for calculating these entropies for arbitrary single and multi-mode Gaussian states, showing how the smoothed version may be calculated numerically. Finally, we demonstrate that when compared to the von Neumann entropy, the min-entropy shows a deviation in the rate of equilibration when considering a simple thermalising system.

6.2 Thermalisation

In quantum systems, the concept of thermalisation involves a number of subtleties not present in the classical description. Most notable, is the fact that unitary evolution of the system as a whole requires that a subsystem must itself keep evolving. This in turn implies continual fluctuations and so the notion of a true steady state becomes unclear. In order to make sense of what we mean by thermalisation, we must first make clear the criteria against which we intend to judge. A convenient set, and those that we shall adopt in this chapter, is provided in the approach by [11, 54].

Given a large quantum system described by a Hilbert space $\mathcal{H}$, and a decomposition $\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_B$, partitioning the system into a subsystem $\mathcal{H}_S$ and bath $\mathcal{H}_B$ and with dimensions $d_S \ll d_B$ respectively we say the subsystem thermalises if the following hold: 1) Equilibration: the system evolves to some steady state, and remains there for almost all times. 2) Independence of the exact initial state of the bath, with the only dependence being on macroscopic quantities such as temperature. 3) Independence of the initial state of the subsystem and

4) The equilibrium state of the subsystem should have a Boltzmannian form, $\rho_S = \frac{1}{Z} \exp(-\frac{H_S}{T})$ (where here H_S is the system Hamiltonian and Z the partition function).

Denoting the global pure state of the system at time t as $|\Psi(t)\rangle$, we can write the density matrix as $\rho(t) = |\Psi(t)\rangle\langle\Psi(t)|$, then the subsystem and bath are found by tracing over their respective counterparts, $\rho_S(t) = \text{Tr}_B \rho(t)$ and $\rho_B(t) = \text{Tr}_S \rho(t)$. The equilibrium state is then defined as the time average of the system, ω ,

$$\omega := \langle \rho(t) \rangle_t = \lim_{\tau \rightarrow \infty} \frac{1}{\tau} \int_0^\tau \rho(t) dt. \quad (6.2)$$

Similarly, we can define ω_S and ω_B as the time averages, or steady states, of the subsystem and bath respectively. For a state to reach equilibrium (and stay close to it for almost all times) we require the time average of the distance between the system state $\rho_S(t)$ and the equilibrium state to be small. In order for this to happen, we require that the number of states that the subsystem can evolve through is small in comparison to the total number of states accessible for the entire system. If we now make the further assumption that the Hamiltonian possess non-degenerate energy gaps, then the total number of accessible states can be expressed as the effective dimension, $d^{\text{eff}}(\omega)$ [54],

$$d^{\text{eff}}(\omega) = \frac{1}{\text{Tr}(\omega^2)}. \quad (6.3)$$

This measure is equal to the inverse purity, or thought of another way, we can write $d^{\text{eff}}(\omega) = 2^{H_2(\omega)}$, where $H_2(\omega)$ is the Rényi entropy of order 2 (see Section 6.3). To quantify how close the system state is to equilibrium, we use the trace distance $D(\bar{\rho}, \rho) = \frac{1}{2} \text{tr}|\bar{\rho} - \rho|$, where $|A| \equiv \sqrt{AA^\dagger}$. By making these general assumptions, Linden *et al.* were able to show that almost any subsystem interacting with a large enough bath will satisfy criteria 1-3). More specifically, they proved the bounds [54],

$$\langle D(\rho_S(t), \omega_S) \rangle_t \leq \frac{1}{2} \sqrt{\frac{d_s}{d^{\text{eff}}(\omega_B)}} \leq \frac{1}{2} \sqrt{\frac{d_s^2}{d^{\text{eff}}(\omega)}}. \quad (6.4)$$

Thus, we see that the relevant measure for determining whether a system will contain subsystems that will equilibrate is related to the purity, which itself is related to the Rényi entropy.

6.3 Min- and Max-Entropies

Consider the Shannon entropy for a random variable X with outcomes $\{x_i : i = 1, \dots, n\}$,

$$H(X) = - \sum_i^n p(x_i) \log p(x_i). \quad (6.5)$$

This quantity gives a measure of the uncertainty in the outcome of performing an experiment, where the probabilities of obtaining the result x_i is given by $p_i = p(x_i)$. One can characterise this function, axiomatically, following Fadeev, [51]

1. $H(X)$ is symmetric in its variables for $n > 1$.
2. $H(p, 1 - p)$ is a continuous function for $0 \leq p \leq 1$.
3. $H(1/2, 1/2) = 1$.
4. $H(tp_1, (1 - t)p_1, p_2, \dots, p_n) = H(p_1, \dots, p_n) + p_1 H(1, 1 - t)$ for any distribution and $0 \leq t \leq 1$.

By relaxing the fourth postulate, and instead replacing it with the weaker requirement that entropy is additive $H(XY) = H(X) + H(Y)$, then (6.5) is no longer the only quantity satisfying the four (new) conditions. One such class of functions is given by,

$$H_\alpha(X) = \frac{1}{1 - \alpha} \log_2 \left(\sum_{k=1}^n p_k^\alpha \right), \quad (6.6)$$

for $\alpha > 0$ and $\alpha \neq 1$. The family (6.6) are called the Rényi entropies of order α , and using L'Hôpital's rule it is straightforward to show that in the limit $\alpha \rightarrow 1$

we recover the Shannon entropy,

$$\lim_{\alpha \rightarrow 1} H_\alpha(X) = - \sum_i^n p(x_i) \log p(x_i). \quad (6.7)$$

For higher values of α the Rényi entropy becomes increasingly dominated by the higher probability events, while for lower values, their weightings become more uniform, independent of their probabilities. In the respective limits we then have,

$$\begin{aligned} H_0 &\equiv \lim_{\alpha \rightarrow 0} H_\alpha(X) = \log |X|, \\ H_\infty &\equiv \lim_{\alpha \rightarrow \infty} H_\alpha(X) = -\log \sup p_i. \end{aligned} \quad (6.8)$$

Rényi entropies also satisfy $H_{\alpha'} \leq H_\alpha$ for $\alpha \leq \alpha'$ and so these values quantify the maximum and minimum values the entropies can take. As such they are often referred to as the max- and min- entropies. Just as the Shannon entropy has its quantum analogue in the von Neumann entropy, the Rényi entropies also have their density matrix equivalents. Correspondingly, the (unconditional) min- and max-entropies are then defined as,

$$H_{\min}(\rho) = -\log \lambda_{\max}, \quad (6.9)$$

$$H_{\max}(\rho) = \log \mathbf{rank}(\rho). \quad (6.10)$$

In the case of a flat distribution, the three measures give the same value.

6.3.1 Smooth min- and max- entropies

The min- and max- entropies are discontinuous and so we can instead define smoothed versions as follows. First we consider the set of all density operators within the open ball ϵ close to ρ , $\mathcal{B}^\epsilon(\rho)$, that is all operators $\bar{\rho}$ such that $\|\bar{\rho} - \rho\| \leq \epsilon$. Here we take the norm to be the trace distance, $D(\bar{\rho}, \rho) = \frac{1}{2} \text{tr} |\bar{\rho} - \rho|$, where

$|A| \equiv \sqrt{AA^\dagger}$. We then define the ϵ -smooth min- and max- entropies as

$$H_{\min}^\epsilon(\rho) = \sup_{\bar{\rho} \in \mathcal{B}^\epsilon(\rho)} H_{\min}(\bar{\rho}), \quad (6.11)$$

$$H_{\max}^\epsilon(\rho) = \inf_{\bar{\rho} \in \mathcal{B}^\epsilon(\rho)} H_{\max}(\bar{\rho}). \quad (6.12)$$

An important property to note is that both measures are unitarily invariant.

6.4 Entropies of Gaussian states

We now provide simple expressions for calculating the entropies of Gaussian states. As a notational convenience, we shall write $H(\gamma) = H(\rho(\gamma))$ when it is understood that the density matrix is described by a covariance matrix γ . These expressions rely explicitly on the following observation. Given any Gaussian state, the covariance matrix γ , describing the expectations of its second moments (3.15) can be diagonalised by way of an appropriate symplectic transform $S \in S_p(2N, \mathbb{R})$,

$$S\gamma S^T = \bigoplus_{i=1}^N s_i \mathbb{I}_2, \quad (6.13)$$

where the $s_i, i = 1 \dots N$, are the symplectic eigenvalues, corresponding to the positive eigenvalues of $i\sigma\gamma$. The matrix $S\gamma S^T$ is then the covariance matrix of N decoupled oscillators, each in a thermal state with mean photon number given by $\bar{n} = (s_i - 1)/2$. Now, by the Stone-von Neumann theorem, symplectic transforms in the phase space Ξ become unitary operators acting on the Hilbert space $\mathcal{H}$, and so we can ignore the transforms in (6.13) when considering operations which are unitarily invariant, such as the von-Neumann and smooth min- and max-entropies. Thus, it suffices to consider only the density matrix for the thermal state described by the symplectic eigenvalues s_i .

6.4.1 Von-Neumann entropy of an N -mode Gaussian state

It follows, that any single mode Gaussian state ρ can be written in the form [61]

$$\rho = U(r, \phi) \nu_s U^\dagger(r, \phi), \quad (6.14)$$

where ν_s is a thermal state with mean photon number $\bar{n} = (s - 1)/2$ and is given by,

$$\nu_s = \frac{2}{1+s} \sum_{k=0}^{\infty} \left(\frac{s-1}{s+1} \right)^k |k\rangle \langle k|. \quad (6.15)$$

For completeness, the operators $U(r, \phi)$ are the single mode squeezing operators $U(r, \phi) = \exp(\frac{1}{2}e^{-i2\phi}a^2 - \frac{1}{2}e^{i2\phi}a^{\dagger 2})$, however as they are unitary they play no role in calculations of the von-Neumann entropy (or smooth entropies). While the corresponding terms in the multi-mode case are not simple tensor products of single mode squeezing operators, they too are unitary, and so henceforth, we shall ignore these terms.

The von-Neumann Entropy for a single mode Gaussian state is given by the following [62, 61]

$$H_v(\gamma) = \left(\frac{s+1}{2} \right) \ln \left(\frac{s+1}{2} \right) - \left(\frac{s-1}{2} \right) \ln \left(\frac{s-1}{2} \right). \quad (6.16)$$

Now, noting the above, that any multi-mode Gaussian state can be decomposed, up to some overall unitary operation, into decoupled thermal modes, we can write $\rho_{\mathbf{mm}} = U_{\mathbf{mm}} (\bigotimes_{k=1}^N \nu_{s_k}) U_{\mathbf{mm}}^\dagger$ ¹. Then using the fact that the von-Neumann entropy is additive on tensor product states, we have the following expression for the von-Neumann entropy of a general Gaussian state [61]

$$H_v(\gamma) = \sum_{k=1}^N f(s_k), \quad (6.17)$$

¹any symplectic transforms $S_{\mathbf{mm}}$ on an N -mode state can be decomposed as $S = O_1 D O_2$, where the O_i generate N -mode rotations, and $D = \mathbf{diag}(k_1, 1/k_1, \dots, k_N, 1/k_N)$ can be interpreted as the single mode squeezings.

where $s = s(\gamma)$ implicitly, and

$$f(s) = \left(\frac{s+1}{2}\right) \ln \left(\frac{s+1}{2}\right) - \left(\frac{s-1}{2}\right) \ln \left(\frac{s-1}{2}\right). \quad (6.18)$$

6.4.2 Smooth min-entropy of a Gaussian state

For the min-entropy, $H_{\min}(\gamma)$, the situation is considerably easier as this relies only on the largest eigenvalue of ρ . Taking the matrix $S\gamma S^\dagger$ to correspond to a single thermal mode, then from (6.15) the eigenvalues of the density matrix in the number state basis are

$$\lambda_n = \frac{(\bar{n})^n}{(1 + \bar{n})^{n+1}} = 2 \frac{(s-1)^n}{(s+1)^{n+1}}. \quad (6.19)$$

Under the transform (6.13), the density operator decomposes into a tensor product of N single mode Gaussian states

$$U^\dagger \rho U = \otimes_{j=1}^N \nu_j, \quad (6.20)$$

where ν_j are the thermal states (6.13). The eigenvalues for the N -mode state ρ , labelled by the occupation numbers of each mode $n_j = 0, \dots, \infty$ are then

$$\lambda_{n_1, n_2, \dots, n_N} = \prod_{j=1}^N 2 \frac{(s_j-1)^{n_j}}{(s_j+1)^{n_j+1}}. \quad (6.21)$$

To calculate the min-entropy we want to find the maximum eigenvalue and so we set each $n_j = 0$. Then we have $\lambda_{\max} = \prod_{j=1}^N \frac{2}{s_j+1}$ and so,

$$H_{\min}(\gamma) = \sum_{k=1}^N g(s_k), \quad (6.22)$$

where

$$g(s) = \log \left(\frac{s+1}{2} \right). \quad (6.23)$$

For the case of the smooth-entropy, we have a little more work. To make

things simpler, let us first consider again a single-mode Gaussian state. Note that as this is unitarily equivalent to a thermal state, it implies $s \geq 1$, and so the eigenvalues of the density matrix are always decreasing and the expression (6.19) is already ordered. The next step is to find a suitable ansatz for the form of the state ρ' which has the minimum largest eigenvalue among all states within ϵ of ρ . This is afforded by the following proposition:

6.4.1. PROPOSITION. *Let λ be the eigenvalues of the state ρ , then there exists a state $\bar{\rho}$ which has the smallest maximum eigenvalue of any state within an open ball $\mathcal{B}^\epsilon(\rho)$ (under the trace distance), and also commutes with ρ . That is, if λ' are the eigenvalues of $\bar{\rho}$ then*

$$\sum_i^\infty |\lambda_i - \lambda'_i| \leq 2\epsilon. \quad (6.24)$$

Proof. Consider a state $\sigma \in \mathcal{B}^\epsilon(\rho)$, such that

$$D(\rho, \sigma) \equiv \frac{1}{2} \text{tr}|\rho - \sigma| \leq \epsilon, \quad (6.25)$$

where $|A| \equiv \sqrt{AA^\dagger}$. We can diagonalise the density matrix ρ with an appropriate unitary transform U , $\nu = U^\dagger \rho U = \sum \lambda_i |i\rangle\langle i|$. The trace distance is preserved under unitary transformations, so applying the transform $\bar{U} = U^\dagger$ to both states, we have

$$D(\nu, \bar{U}\sigma\bar{U}^\dagger) = D(\rho, \sigma) \leq \epsilon, \quad (6.26)$$

that is, there is a state $\bar{\sigma} = \bar{U}\sigma\bar{U}^\dagger$ within ϵ of ρ . What remains is to show that for any $\bar{\sigma}$ there is a related diagonal state $\bar{\rho}$ with $\lambda_{\max}(\bar{\rho}) \leq \lambda_{\max}(\bar{\sigma})$, which is also within trace distance ϵ of ρ . This can be accomplished using the pinching inequality [63],

$$|||\mathcal{C}(A)||| \leq |||A|||, \quad (6.27)$$

where $|||\cdot|||$ is any unitarily invariant norm, and the pinching operator $\mathcal{C}(A)$ sets off diagonal entries to zero². What holds for any unitarily invariant norm, must

²The pinching operator is defined as $\mathcal{C}(A) = \sum_{j=1}^k P_j A P_j$, where $P_1, \dots, P_k$ are mutually

then hold for the operator norm (Ky Fan 1-norm), $\|A\| = \Sigma_1(A)$ where $\Sigma_1(A)$ is the largest singular value of A , and so for a matrix A , the largest eigenvalue never increases under pinchings. The final step is to note that the pinching operator is a trace preserving operation and so, setting $A = \bar{\sigma}$, we have

$$D(\mathcal{C}(\nu), \mathcal{C}(\bar{\sigma})) = D(\nu, \bar{\rho}) \leq \epsilon, \quad (6.28)$$

□

Therefore, in order to calculate the smooth min-entropy we need to find the largest eigenvalue from the set $\{\lambda'_{\max}\}$ such that

$$\sum_i^{\infty} |\lambda_i - \lambda'_i| \leq 2\epsilon. \quad (6.29)$$

The left hand side has infinitely many terms, however we can perform the minimisation by first assuming $\lambda'_i = \lambda_i, \forall i$ and then shifting only the largest m unprimed eigenvalues such that their new average, shifted by ϵ/m is larger than the $m + 1^{\text{th}}$ eigenvalue³. To preserve the trace, we must then add an amount ϵ to the smallest eigenvalues, however, as the system is infinite dimensional, we can spread this extra contribution over an infinite number of eigenvalues, and so $\lambda'_m = \lambda_m > \lambda'_{m+j}, \forall j$. Thus we need to find the maximum eigenvalue

$$\lambda'_{\max} = \max_m \left\{ \frac{(\sum_{i=0}^{m-1} \lambda_i) - \epsilon}{m} \left| \frac{(\sum_{i=0}^{m-1} \lambda_i) - \epsilon}{m} \geq \lambda_m \right. \right\}. \quad (6.30)$$

As the $\{\lambda_i\}$ are an ordered set, substituting (6.19) we need the maximum m such that

$$1 - \left(1 + \frac{2m}{s+1}\right) \left(\frac{s-1}{s+1}\right)^m \leq \epsilon. \quad (6.31)$$

orthogonal projections.

³Recall that the eigenvalue labelling begins at zero.

Multi-mode Gaussian states

The computational ease of the single mode smoothed min-entropy above relies on the fact that (6.19) is already ordered. Unfortunately the extension to the multi-mode case is complicated by the dependence on relations between symplectic eigenvalues. A brute force numerical ordering would run into difficulties given the infinite dimension of the Hilbert space, however we can effectively truncate the dimension by placing crude limits on the relevant occupation numbers in (6.21). This then restricts the number of eigenvalues which need to be ordered “by hand”. It is clear that the largest eigenvalue will be that with all occupation numbers set to zero. We also know that the the minimum eigenvalue we need to consider, $\lambda_{\bar{m}}$ ($\bar{m} = m_1 \cdots m_N$), is smaller than the maximum by at most ϵ . Now, by considering in turn each occupation number, while all others are held at zero, we can put limits on the number of possibly relevant terms, which can then be ordered computationally.

For simplicity let us first call the normalisation factors associated to the various modes $C = \prod_j^N 2/(s_j + 1)$, with the remaining occupation number dependent terms $a_j = \left(\frac{s_j-1}{s_j+1}\right)$. Then

$$\lambda_{\bar{m}} \geq \lambda_{\max} - \epsilon = C - \epsilon. \quad (6.32)$$

Fixing all $n_k = 0, k \neq j$,

$$\begin{aligned} C a_j^{m_j} &\geq C - \epsilon, \\ \implies \lambda_{\max}(1 - a_j^{m_j}) &\leq \epsilon, \end{aligned} \quad (6.33)$$

and so a crude upper bound on each occupation number is

$$m_j = \left\lfloor \frac{\log\left(1 - \frac{\epsilon}{\lambda_{\max}}\right)}{\log \frac{s_j-1}{s_j+1}} \right\rfloor. \quad (6.34)$$

This only holds so long as $\lambda_{\max} > \epsilon$, and so for large N or s_j (i.e. T) we must be

careful in our choice of smoothing.

6.4.3 Smooth max-entropy

Single mode Gaussian state

From (6.19) it is clear that the rank, and hence the max-entropy are divergent for a general Gaussian state when any of the symplectic eigenvalues take the value $s_j > 1$. However, it turns out that it is still possible to find a state nearby (i.e. ϵ -close) which is non-Gaussian and has finite rank. This allows one to make sensible use of the smooth-max entropy. However, as before, in order to simplify the minimisation we need a statement akin to Prop. 6.4.1. This is afforded by the following

6.4.2. PROPOSITION. *Let λ be the eigenvalues of the state ρ , then there exists a state $\bar{\rho}$ which has the smallest rank of any state within an open ball $\mathcal{B}^\epsilon(\rho)$ (under the trace distance), and also commutes with ρ . That is, if λ' are the eigenvalues of $\bar{\rho}$ then*

$$\sum_i^\infty |\lambda_i - \lambda'_i| \leq 2\epsilon. \quad (6.35)$$

Proof.

The proof follows quite straightforwardly from an inequality by Mirsky [64, 63],

$$|||\mathbf{Eig}^\downarrow(A) - \mathbf{Eig}^\downarrow(B)||| \leq |||A - B|||, \quad (6.36)$$

which holds for all unitarily invariant norms and Hermitian matrices, A and B , with $\mathbf{Eig}^\downarrow(A)$ the diagonal matrix whose diagonal entries are the (decreasing) eigenvalues of A . Take σ to be the state in $\mathcal{B}^\epsilon(\rho)$ with minimum rank, and consider the basis where ρ has been diagonalised and ordered. Then from the above inequality

$$|||\nu - \mathbf{Eig}^\downarrow(\sigma)||| \leq |||\rho - \sigma||| \leq \epsilon. \quad (6.37)$$

However $\mathbf{Eig}^\downarrow(\sigma)$ is just the state, which we will call $\bar{\rho}$, which is diagonal in the same basis as ρ , and so by the above inequality this must also lie in $\mathcal{B}^\epsilon(\rho)$. As

the rank only depends on the eigenvalues, this proves the theorem. $\square$

In fact, the same argument can equally be applied to Prop. 6.4.1, and so we extend Proposition 6.4.2 to include both:

6.4.3. PROPOSITION. *given a state ρ , then for any state σ within a ball $\mathcal{B}^\epsilon(\rho)$, there exists another state $\sigma' = \mathbf{Eig}^\downarrow(\sigma) \in \mathcal{B}^\epsilon(\rho)$ which is diagonal in the same basis as ρ .*

We can now explicitly construct a state with minimum, finite rank by first noting that $\mathbf{tr}(\rho) = 1$, and that (6.19) is strictly decreasing for all $s_j > 1$. Together these imply that for any $\epsilon > 0$ there will be a finite number of terms such that $\sum_i \lambda_i \geq 1 - \epsilon$. Thus, using condition (6.24) we begin by assuming $\lambda' = \lambda$, and then set $\lambda'_{i>m} = 0$, for some finite m . This corresponds to the tail $\sum_{i=m+1}^\infty \lambda_i \leq \epsilon$. To preserve the trace, we must also include an additional ϵ contribution to the sum of largest $m + 1$ eigenvalues, however as the rank is unaffected by the the magnitude of the eigenvalues, the manner in which this is done is unimportant. Thus,

$$\sum_{i=m+1}^\infty \lambda_i = 1 - \sum_{i=0}^m \lambda_i \leq \epsilon. \quad (6.38)$$

Substituting (6.19), we have

$$\begin{aligned} 1 - \frac{2}{s+1} \sum_{j=0}^m \left(\frac{s-1}{s+1} \right)^j &\leq \epsilon \\ \left(\frac{s-1}{s+1} \right)^{m+1} &\leq \epsilon, \end{aligned} \quad (6.39)$$

and so

$$m + 1 = \mathbf{rank} = \left\lceil \frac{\log \epsilon}{\log \frac{s-1}{s+1}} \right\rceil, \quad (6.40)$$

where the ceiling function $\lceil x \rceil$ is the smallest integer not less than x . For single mode Gaussian states, the smooth max-entropy is then given by,

$$H_{\max}^\epsilon(\rho) = \log \left(\left\lceil \frac{\log \epsilon}{\log \frac{s-1}{s+1}} \right\rceil \right). \quad (6.41)$$

Multi mode Gaussian state

For larger subsystems the smooth max-entropy needs to be calculated numerically. However, this poses far greater challenges than for the smooth min-entropy, as now we are interested in the tail of the distribution and so must sum eigenvalue contributions leading to $1 - \epsilon$. On the other hand, for equilibration rates the quantity of interest is the min-entropy, and so our simulations will not include $H_{\max}^\epsilon$. We note, however, that for some applications this numerical difficulty could pose problems.

6.5 Numerical Modeling

Using the tools developed above, we now test our hypothesis that the min-entropy is in some sense the appropriate measure for studying the thermodynamics of small quantum systems. In particular, we wish to show that typical von Neumann entropy is a less reliable (albeit this is small) indicator of equilibration. One may already anticipate that this may be true from the appearance of the Rényi entropy $H_2(\rho)$ in (6.4), however in that case the effective dimension is that of the bath (or, for the weaker bound, the system as a whole), and not the subsystem directly. For that, we provide the following motivation by considering the end points of the system described below.

Consider N two level systems in a mixed state, where with probabilities p and $(1 - p)$ the system is in a thermal (Gibbs) state of temperatures T_1 and T_2 respectively. This system is then brought into contact with a bath of size M at temperature T_B and left to equilibrate. Initially, we have the total state

$$\rho^i = [p(\rho_s(T_1)^{\otimes N}) + (1 - p)(\rho_s(T_2)^{\otimes N})] \otimes \rho_b(T_B)^{\otimes M}, \quad (6.42)$$

where we use the upper and lower case latin alphabet to denote the partitioned systems and the individual components within them, i.e. ρ_s refers to a single two

level system within the subsystem ρ_S . The thermal (Gibbs) state is given by

$$\rho_s(T) = \frac{\exp\left(-\frac{H}{k_B T}\right)}{Z} = \frac{1}{Z} \begin{pmatrix} 1 & 0 \\ 0 & e^{-\frac{1}{k_B T}} \end{pmatrix}, \quad (6.43)$$

where the Hamiltonian for each component system (qubit) is given by $H = |1\rangle\langle 1|$ and $Z = 1 + e^{-\frac{1}{k_B T}}$ is the partition function. Now if the bath is suitably large, we can expect that the final state is, to a good approximation, that of the thermal state at the temperature of the bath,

$$\rho_S^f \approx \rho_S(T_B)^{\otimes N}. \quad (6.44)$$

Taking the extremal case $T_1 = 0$ and $T_2 = \infty$ (i.e. that the initial subsystem is either very hot, or at zero temperature) and substituting (6.43) into (6.42) and (6.44) respectively we can calculate the values of the min- and von Neumann entropies for the initial and final states. We have then,

$$\begin{aligned} H_{\min}(\rho_S^i) &= -\log \lambda_{\max} = -\log \left(1 - p \left[1 - \frac{1}{2^N} \right] \right), \\ H(\rho_S^i) &= -\text{Tr}(\rho_S^i \log \rho_S^i) = - \left(1 - p \left[1 - \frac{1}{2^N} \right] \right) \log \left(1 - p \left[1 - \frac{1}{2^N} \right] \right) \\ &\quad - (2^N - 1) \frac{p}{2^N} \log \left(\frac{p}{2^N} \right). \end{aligned} \quad (6.45)$$

While at the end of the thermalisation,

$$\begin{aligned} H_{\min}(\rho_S^f) &= N \log Z, \\ H(\rho_S^f) &= \frac{N}{Z} \left(\log Z + e^{-\frac{1}{k_B T_B}} \log Z e^{\frac{1}{k_B T_B}} \right). \end{aligned} \quad (6.46)$$

A plot of these values for a subsystem size of $N = 20$ qubits shows that for some values p , the initial and final von Neumann Entropy of the system is the same, while the min-entropy necessarily increases, Fig. 6.1. For a system of 20 qubits, this should happen around $p = 0.7$. While it is true the entropies of the subsystem can both increase and decrease, we should expect that for at least some of the

evolution these entropies should change at different rates. To be certain however, we must keep track of what happens during the entire dynamics, and not just the end points.

However, modeling a qubit system of this size is exceedingly difficult, especially when one includes the effects of the bath, and so we instead try to find an analogous Gaussian system which also displays a similar behaviour. Such a system, along with its bath, can be efficiently modeled either numerically or with simple master equations such as those in Chapter 5.

6.5.1 Harmonic Chain Model

The obvious choice is a mixed N mode thermal Gaussian state, connected to a bath at temperature T_B . Again the initial and final states of the system take the form,

$$\rho_S^i = p\rho_{\text{th}}(N, T_1) + (1 - p)\rho_{\text{th}}(N, T_2), \quad (6.47)$$

$$\rho_S^f \approx p\rho_{\text{th}}(N, T_B), \quad (6.48)$$

but now the N -mode thermal states, $\rho_{\text{th}}(N, T)$, are described by covariance matrix elements (3.17),

$$\gamma_{j,k} = \delta_{jk} \left(1 + \frac{2}{e^{\omega_j/T} - 1} \right). \quad (6.49)$$

In general, however, a mixture of two Gaussian states need not be Gaussian, (see for example [66]), and so the tools we have developed will not apply here⁴. Instead, we note the reliance above on the parameter p in fine tuning the initial state of the system. This suggests that rather than relying on a mixed state, it should be sufficient to split the chain into regions which are initially at different temperatures. We can then tune the system to observe the desired effect.

The model we shall adopt for this system is that of a chain of $N = N_1 + N_2$ harmonic oscillators, coupled to their nearest neighbours in the rotating wave

⁴In fact, for mixtures of thermal states, i.e. those diagonal in the same basis, we can still calculate the min-entropy, however such a state would not remain so throughout the evolution.

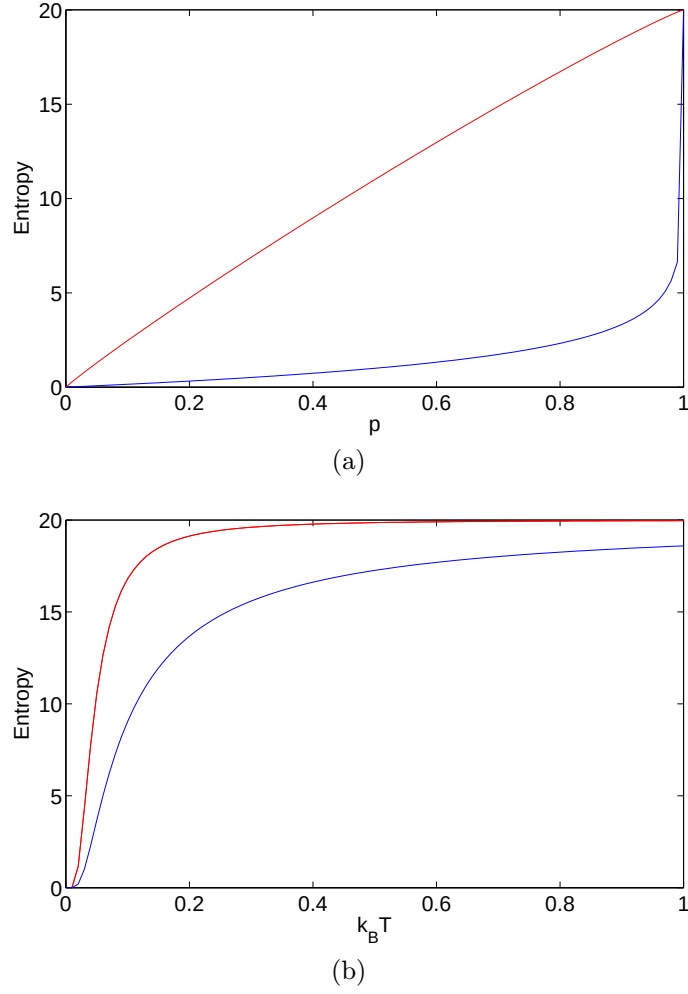


Figure 6.1: Comparisons of the initial and final state entropies. In Fig a) the min entropy (blue) and von Neumann entropy (red) are plotted as a function of the probability p for $N = 20$ qubits, Fig b) shows the final entropies as a function of the bath temperature $k_B T_B$.

approximation. For simplicity, we'll assume that the strength of interaction is the same across the chain, and specified by coupling c . To each oscillator j we then attach a bath, composed of M harmonic oscillators, each coupled with strength $g_{j,k}$. The Hamiltonian for this system is then given by,

$$\begin{aligned}
H = & \sum_j^N \Omega_j a_j^\dagger a_j + \sum_j^{N-1} c_j (a_j^\dagger a_{j+1} + a_j a_{j+1}^\dagger) \\
& + \sum_j^N \sum_k^M \omega_{j,k} a_{j,k}^\dagger a_{j,k} \\
& + \sum_j^N \sum_k^M g_{j,k} (a_j^\dagger a_{j,k} + a_j a_{j,k}^\dagger).
\end{aligned} \tag{6.50}$$

The first line describes the coupled chain, while the two double summation terms in the second and third lines refer to the bath oscillators and their coupling to each of the chain oscillators respectively. Note there is no direct coupling between oscillators in the baths. As it stands, this is still a little too general to properly describe an environment. For that we must make an appropriate choice of the couplings $g_{j,k}$, and we do this by distributing their values according to the desired spectral density $J(w)$ of the baths. Here we take an Ohmic spectral density, see Sec. 5.2.2 [2].

To model the evolution we could choose to re-write the Hamiltonian in terms of the canonical position and momentum operators x and p using the transform Ω as in section 3.3.1. Then all we need do is substitute, using the appropriate matrix description, into the general solution. On the other hand, we can equally start by considering the Hamiltonian (6.50) directly. Working through the calculation explicitly we begin with the Heisenberg equation,

$$\begin{aligned}
i\dot{a}_l &= [a_l, H] = \Omega_l a_l + c_l a_{l+1} + c_{l-1} a_{l-1} \\
&\quad + \sum_k^M g_{l,k} a_{l,k}, \\
i\dot{a}_{l,m} &= [a_{l,m}, H] = g_{l,m} a_l + \omega_{l,m} a_{l,m},
\end{aligned}$$

where $a_0 = a_{N+1} = 0$. To make things easier, we can construct a vector of annihilation operators, $A = (a_1, a_{1,1}, \dots, a_{1,M}, a_2, \dots, a_{N,M})^T$. The Heisenberg equations can then be written in the form of a matrix equation,

$$i\dot{A} = WA, \quad (6.51)$$

where the matrix W is given by

$$W = \begin{pmatrix} \Omega_1 & g_{11} & \cdots & g_{1M} & c_1 & & & & & & \\ g_{11} & \omega_{12} & & & & & & & & & \\ \vdots & & \ddots & & & & & & & & \\ g_{1M} & & & \omega_{1M} & & & & & & & \\ c_1 & & & & \Omega_2 & g_{21} & \cdots & g_{2M} & c_2 & & \\ & & & & g_{21} & \omega_{21} & & & & & \\ & & & & \vdots & & \ddots & & & & \\ & & & & g_{2M} & & & \omega_{2M} & & & \\ & & & & c_2 & & & & \Omega_3 & & \\ & & & & & & & & & \ddots & \\ & & & & & & & & & & \ddots \\ & & & & & & & & & & c_{N-1} & \Omega_N & g_{N1} & \cdots & g_{NM} \\ & & & & & & & & & & & g_{N1} & \omega_{N1} & & \\ & & & & & & & & & & & \vdots & & \ddots & \\ & & & & & & & & & & & g_{NM} & & & \omega_{NM} \end{pmatrix}$$

This is a somewhat sizeable matrix, but it is nevertheless only half the size of that describing the full Hamiltonian. The simplification arises because by using the RWA we neglected terms of the form $a^\dagger a^\dagger$, and so $K^{(c)}$ (defined in Chapter 3) contains no block diagonal components. As a consequence, in the solution for $A^{(c)}(t)$ the creation and annihilation operators do not mix. Furthermore, in order for the Hamiltonian to be Hermitian, the off diagonal components must

be identical. In terms of the canonical operators, this means the kinetic and potential parts of the Hamiltonian are also equal, i.e. $V = T = \frac{1}{2}W$. From the results of Section 3.3.2 we have,

$$R(t) = \mathcal{M}R(0) = \begin{pmatrix} T_R & -T_I \\ T_I & T_R \end{pmatrix} R(0), \quad (6.52)$$

where,

$$\begin{aligned} T_R &= \frac{T + T^\dagger}{2} = \cos(Wt), \\ T_I &= \frac{T - T^\dagger}{2i} = -\sin(Wt). \end{aligned} \quad (6.53)$$

The simple form for this solution arises from the Hamiltonian containing only linear couplings. This fact also means any initial Gaussian state will remain Gaussian throughout the evolution, and so we can restrict our attention to the covariance matrix, $\gamma(t)$. Using the result from section 3.3.1 we have finally,

$$\gamma(t) = \mathcal{M}\gamma(0)\mathcal{M}^T. \quad (6.54)$$

In our model we are only interested in the state, in particular the entropy, of the system and so the environment oscillators can be traced out. Recalling the partial trace property of covariance matrices (3.18), we only need to consider elements corresponding to the oscillators in the chain.

6.5.2 Specifying the initial state

All that is left then is to give the initial state of the covariance matrix $\gamma(0)$. For the above model, this corresponds to the initial system and bath states,

$$\begin{aligned} \rho_S^i &= \rho(T_1)^{\otimes N_1} \otimes \rho(T_2)^{\otimes N-N_1}, \\ \rho_B^i &= \rho(T_B)^{\otimes NM}, \end{aligned} \quad (6.55)$$

where the covariance matrix for a thermal mode is given by (6.49). For our choice of basis we have

$$R = (X_1, X_{1,1}, \dots, X_{1,N}, X_2, \dots, X_{NM}, P_1, P_{1,1}, \dots, P_{1,N}, P_2, \dots, P_{NM})^T, \quad (6.56)$$

Recalling that system oscillators are specified by a single index, R_j , while bath oscillators take on two R_{jk} . As a check it could be worthwhile to compare the final system state to that of a thermal state at temperature T_B .

To get an idea of which parameter values to choose, let us look at the (non-smoothed) min- and von Neumann entropies for the initial and final states. These rely on the three symplectic eigenvalues corresponding to thermal modes at temperatures T_1 , T_2 and T_B . Using equations (6.17) and (6.19) we have,

$$\begin{aligned} H_{\min}(\rho_{sys}^i) &= N_1 \log \left(\frac{s_1 + 1}{2} \right) + (N - N_1) \log \left(\frac{s_2 + 1}{2} \right), \\ H(\rho_{sys}^i) &= N_1 f(s_1) + (N - N_1) f(s_2). \end{aligned} \quad (6.57)$$

where the symplectic eigenvalue for a mode a thermal state is given by

$$s_i = 1 + \frac{2}{e^{\omega_i/K_B T_i} - 1}, \quad (6.58)$$

and the function $f s$ is defined as in (6.18),

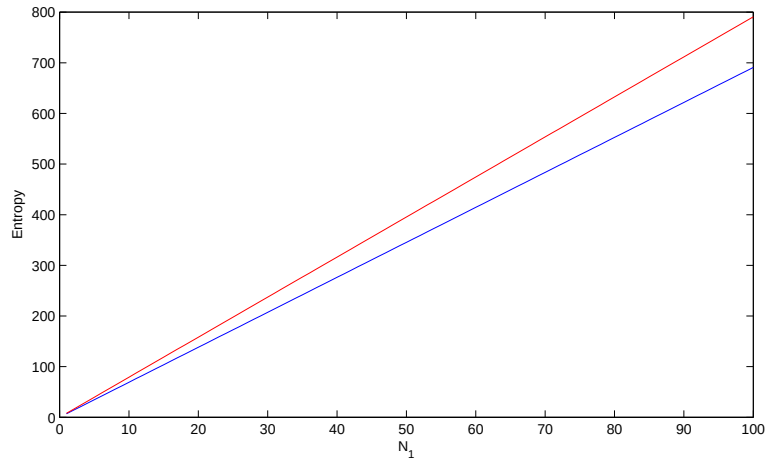
$$f(s) = \left(\frac{s+1}{2} \right) \ln \left(\frac{s+1}{2} \right) - \left(\frac{s-1}{2} \right) \ln \left(\frac{s-1}{2} \right). \quad (6.59)$$

Similarly, for the final state we have,

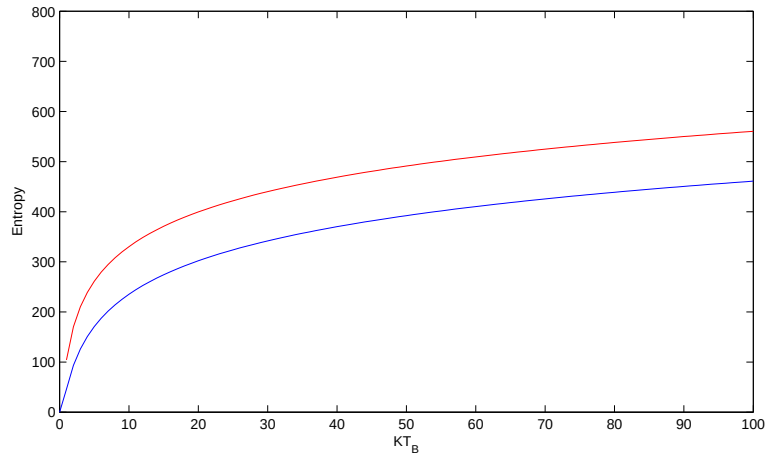
$$\begin{aligned} H_{\min}(\rho_{sys}^f) &= N \log \left(\frac{s_B + 1}{2} \right), \\ H(\rho_{sys}^f) &= N f(s_B). \end{aligned} \quad (6.60)$$

As an example, we plot in Fig 6.2 comparisons of the entropies for the initial and final states as a function of the parameter N_1 and bath temperature T_B

when the system temperatures are $T_1 = 0$ and $T_2 = 1000$. While the difference in behaviour for the two entropies is much less than the case of a discrete mixed initial state, there still appears to a wide range of parameters such that the $H^i = H^f$ and $H_{\min}^i \neq H_{\min}^f$.



(a)



(b)

Figure 6.2: Comparisons of the initial and final state entropies. In Fig a) the min entropy (blue) and von Neumann entropy (red) are plotted as a function of the number of oscillators N_1 at temperature $K_B T = 1000$, while $N - N_1$ oscillators are at $K_B T = 0$. Fig b) shows the dependence on the bath temperature T_B .

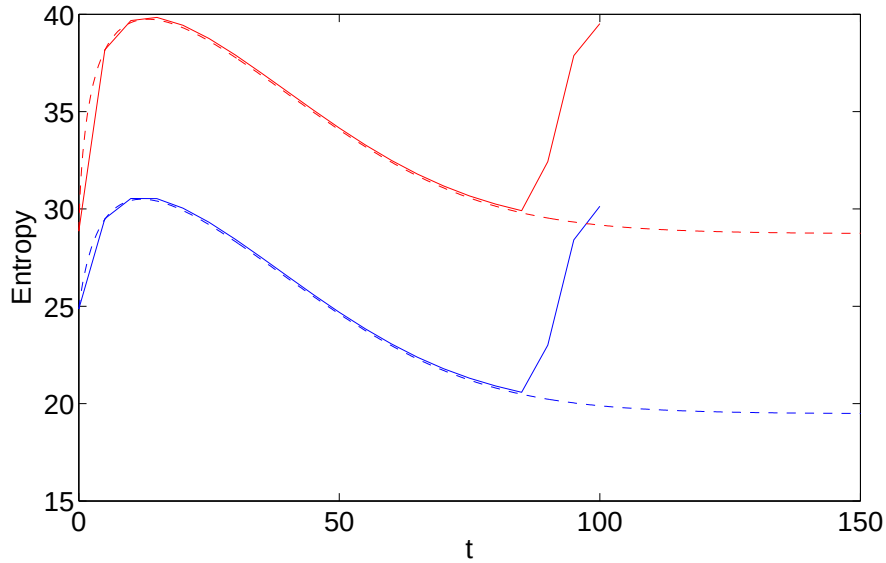


Figure 6.3: The exact evolution of the min- (blue) and von Neumann (red) entropy for a chain of $N = 10$ oscillators, partitioned such that initially $N_1 = 4$ are at temperature $k_B T_1 = 1000$, and $N_2 = 6$ at $k_B T_2 = 0.1$ and each are brought into contact with a bath of $N_{B_i} = 280$ oscillators at temperature $k_B T_B = 13$. Bath and internal couplings are given by $\alpha = 1/100$ and $\beta = 1/500$ respectively. Dashed lines as calculated from a master equation. It is clear that even with a total bath size of $N_B = 2800$ oscillators, revivals still occur before equilibration

6.6 Results

In Fig. 6.3 we plot the evolution of the von Neumann and min entropy as a small chain comes into equilibrium. Note, that even with a bath 280 times larger than the subsystem, simulations do not reach equilibrium before revivals become important at $t_{\text{rev}} \approx 80$. As a comparison, we overlay the results obtained from a straightforward extension to the master equation 5.27, which as argued in Chapter 5 should provide an accurate description in the chosen parameter regime. In fact, we can see at early times $t < t_{\text{rev}}$ this is indeed the case. In general, one should expect both entropy measures to equilibrate exactly when the system is in equilibrium, so instead we plot their respective entropy gradients, Fig 6.4. In plot 6.4a, we see that the gradient for the min entropy lags behind the von Neumann entropy, suggesting it does indeed show a slower approach to equilibrium. Note that while a smaller gradient could be attributed to a respective scaling between

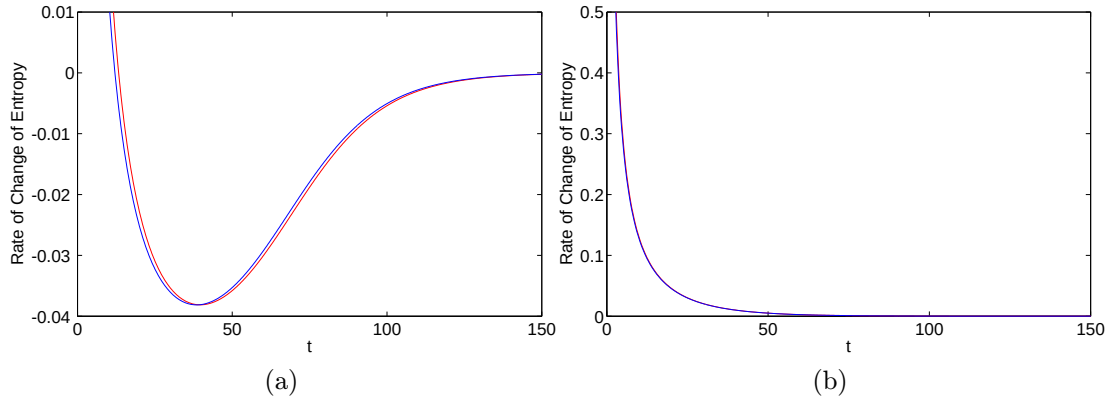


Figure 6.4: Comparisons of the rate of change of the min entropy (blue) and von Neumann entropy (red) as calculated from a master equation with bath coupling $\alpha = 1/100$ and internal coupling $\beta = 1/500$ connected to a subsystem of size $N = 10$. In Fig a) $N_1 = 4$, $k_B T_1 = 1000$, $k_B T_2 = 0.1$ and $k_B T_B = 13$, while in Fig b) . Note in Fig a) our choice of parameters implies $H(\rho_S^i) \approx H(\rho_S^f)$. Only in this plot do we see an appreciable (albeit small) lag in the gradient of the min entropy. In fact, a closer inspection reveals that for both plots, the gradient of min entropy is smaller than that for the von Neumann entropy leading up to the approach to equilibrium

the absolute values of each entropy, the lag here suggests there is a more general slowing of the response.

6.7 Summary and Outlook

In this chapter we have extended the standard formulations of the smooth min- and max- entropies to the case of Gaussian states. While the unsmoothed versions are remarkably easy to calculate - given by either a simple function of the symplectic eigenvalues, (6.22), or in the case of the max-entropy, simply divergent - the smooth versions require more care to be computationally efficient. Nevertheless, we have been able to provide analytic solutions in some cases, and suggested crude bounds to improve efficiency in others.

This has allowed us to gain new insight into the role of entropy measures in tracking the process of thermalisation. The key ingredient being the ability to simulate Gaussian systems efficiently. In particular, we have shown that in

small quantum systems, the min-entropy equilibrates on a slower timescale than the von Neumann entropy, suggesting that this is therefore a more appropriate measure than those usually applied to macroscopic quantities. This observation adds weight to the argument that one should instead consider the min-entropy when formulating thermodynamics for mesoscopic systems. Of course, it is then natural to ask what role can be played by other Rényi entropies, especially given the bound by [54] (6.4), and a first step in this direction would be to formulate expressions for the Rényi entropies of Gaussian states. One may also ask the reverse question, can we find a similar bound based on the min-entropy?

In Section 6.5.2 we noted that while there was still a deviation in the qualitative behaviour of the min- and von Neumann entropies, this was not as pronounced as with the mixed state case. It would therefore be of interest to extend our analysis to find systems with larger discrepancies. However, the inference here is that doing so would require an extension to (at least a restricted class of) non-Gaussian states. In fact, it may turn out that the min-entropy may be a tractable measure in these circumstances, given we are only interested in the largest eigenvalue of the density matrix. Indeed, for some very restricted cases, it is easy to calculate the min-entropy. An example of this is when a mixture of two Gaussian states is diagonalizable in the same basis (e.g. a classical mixture of thermal states), in which case the equation for a single mode mixture is given by,

$$H_{\min}(\rho_S^i) = pN \log \left(\frac{s_{T_1} + 1}{2} \right) + (1-p)N \log \left(\frac{s_{T_2} + 1}{s_{T_1} + 1 + p(s_{T_2} - s_{T_1})} \right). \quad (6.61)$$

where s_{T_1} and s_{T_2} are the symplectic eigenvalues for thermal modes at temperature T_1 and T_2 respectively. Generalising this extension could lead to interesting further work.

7.1 Summary

Random processes are ubiquitous in all areas of physics. They lie at the heart of quantum mechanics, and yet act as a constant impediment to the implementation of any quantum technology. Despite this, we have seen that randomness (if suitably uniform) can actually have practical benefits, and one can envisage that random quantum operators could play as important a role for quantum computing as random numbers do in classical computers.

Understanding efficient, and convenient methods for generating them is thus a worthwhile objective. Of course, truly random operations, at least in the sense discussed in Chapter 2, cannot hope to be efficient. Nevertheless, downgrading this requirement to pseudo random operators can still be of use, and indeed this thesis has demonstrated a scheme which appears, very strongly, to be both efficient and asymptotically random. What makes this approach unique however, is that it is contained within an entirely quantum framework. That is there is no external classical input of randomness, whether from a quantum source or otherwise.

In Chapter 5 we derived a number of different Markovian master equations for

harmonic systems. The advantage of this is that such models can be efficiently simulated using Gaussian states, and so one can accurately test the validity of the assumptions made in derivation process. In particular, we have shown that common statements regarding the deficiencies of these equations at low temperature need not be warranted. In fact, the Markovian master equations studied here provide a good description of the true dynamics, regardless of the temperature of the bath.

On the other hand, for extended systems we typically must resort to complementary approaches when looking for a Markovian description. This stems from the need to make assumptions regarding the dominant coupling strengths, that is, whether they are within the system or externally to the bath. An important question is then how well each description works as we transition between the two regimes. Again, by using Gaussian systems, we have been able to explore this issue in detail. We find that the two approaches compliment each other well, and so by using both equations one can accurately describe the evolution across all but a small section of the coupling parameter regime. More surprisingly however, is that if the components of the system share a common bath (or rather baths at the same temperature) then either approach works well quite generally.

Finally, the study of master equations transition quite naturally into thermodynamics. Indeed, almost without exception, an open system (and in fact, a suitably large closed system) will evolve into an equilibrium state. In many cases this will be thermal. One is then typically interested in relating macroscopic properties to measures of the microscopic system. In most instances one would choose the von Neumann entropy, but this is by no means the only possibility. In fact, for some situations, another set of entropy measures may be more relevant. These are known as the smooth min and max entropies. However, to what extent this may or may not be true is not well understood. To explore these ideas however, one is naturally lead to continuous variable systems, and in particular, those which are also Gaussian. As a first step we have derived expressions for evaluating these measures when applied to Gaussian states. This then allowed us to examine questions of thermalisation, and in particular we were able

to compare how accurately these measures tracked the approach to equilibrium. Here, results suggest the min entropy records a slower approach and so we can tentatively suggest this may be the most appropriate measure in such cases.

7.2 Outlook

The work in this thesis suggests many further avenues of research. For completeness, the most pressing of these is the desire to prove universality in the scheme presented in Chapter 2. While the analysis strongly suggested this to be the case, it nevertheless rested on numerical results. This leaves a somewhat unsatisfactory feeling, and puts the approach at a distinct disadvantage when compared to other proposals. In fact such a proof may have additional benefits. One could imagine that understanding precisely why this scheme is universal (if indeed it is so) would give a better insight into how the space of operators is explored. In particular, this may suggest clues as to how one can optimise the convergence rates. Indeed, we have already seen that by controlling the ϕ parameter one can speed up or slow down the randomisation process, however, as yet there is no explanation as to why an optimum appears at around $\phi = 5\pi/8$. Indeed, even without a rigorous proof, it is still natural to ask how the speed, and scaling compare to proposals already in the literature.

On the topic of master equations, a number of interesting questions remain. A key motivation was to explore the regimes of applicability when describing an extended test system. While the two approaches studied complement each other quite well, there is still a small but important parameter space where both are seen to break down. In particular, when the internal and external couplings are comparable. A natural question is then how to derive an acceptable Markovian master equation in this case? Interestingly one possibility may be to relax the secular approximation, and for the coupled two oscillator system early results have shown this to be exceptionally promising. Unfortunately, one can no longer guarantee complete positivity, and so understanding under what circumstances this approach is still acceptable is of great interest. Indeed, it is reassuring to note

(Appendix 5.A.3) that a completely positive equation can sometimes be achieved even without taking this approximation.

Of course, Markovian equations are not the only relevant master equations, and so extending this study into the non-Markovian realm may also be of interest. Again, by restricting the systems of interest to harmonic oscillators, exact dynamics can be simulated.

In the last chapter the most speculative work was presented, and it is therefore unsurprising that much can still be done. Notably, it would be desirable to make a concrete demonstration of a difference in behaviour between the (smooth) min and von Neumann entropy. One possibly route would be to study the dynamics of (slightly) non-Gaussian states. Inevitably this would require the development of a number of new techniques, however this in itself would be of interest. Particularly as the availability of usable entropy measures (in a practical sense) for non-Gaussian states is somewhat lacking.

Appendix A

Notation

General

$\log$	binary logarithm
$\ln$	natural logarithm
e	Euler's constant
$\mathbb{E}(X)$	expectation value of random variable X
$\lim$	limit
$\min$	minimum
$\max$	maximum
$\sup$	supremum
$\inf$	infimum
$\text{poly}(n)$	a polynomial in n (determined from the context)

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